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Component Description of Sediment-Water Microcosms

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COMPONENT DESCRIPTION OF SEDIMENT-WATER MICROCOSMS

by

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ABSTRACT

The development and application of complementary variables (potential and flux) for modeling environmental systems are illustrated for the hydraulic and dissolved oxygen subsystems of laboratory microcosms. These sediment-water, semi-continuous flow microcosms were used to determine nutrient interchange and mercury interactions under lighted (aerobic) and dark (anaerobic) conditions. The approach of using complementary variables to describe such systems forces a more complete conceptual understanding of the system and better attention to those parameters (many of which are unknown) requiring measurement.

Complementary variables are incorporated into basic linear component equations which describe basic processes of energy transfer and transformation. The components are interconnected through the use of bond graphs and reduced through topographic and matrix techniques to state space system equations. A transfer function is determined from the state equations and from time domain analysis of the system output. These two expressions of the transfer functions are used to determine component values.

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

INTRODUCTION

Man's Interaction with Ecosystems

By application of increasing technological capability to the use of energy resources, man has become more important in global ecology as a force of geological magnitude than as a biological force. The negative feedback controls or homeostatic mechanisms which have evolved in ecological systems cannot cope with many of man's activities (Odum, 1971). To stem the growing environmental crisis man must become self-regulating with respect to population and industrial growth which affect the environment.

Effective self-regulation requires an operational description of the environment. The environment is a collection of biological, chemical, and physical components which, as Commoner (1973, p. 33) states, "Everything is connected to everything else." A system is a set of interacting components and the environment is a system. Systems analysis, a mathematical description of system behavior, can provide an operational description of the environment which may be used to develop controls to regulate man's interaction with the environment.

Problems in Systems Analysis of Ecosystems

Most system analyses of large ecological or environmental systems are based upon compartment models (Walters, 1971). The principle classes of variables in these models are (1) the fluxes or rates of flow, (2) the state variables or storage levels in each compartment, (3) the inputs or forcing functions, and (4) the parameters which multiply the state variables and inputs. There are no explicit potentials or forces which cause the flows in these models.

The potentials associated with the fluxes in these models are incorporated into the parameters which modify the state variables. In the usual method of development these parameters also include many of the effects of environmental interaction with the compartment. As explained by Walters (1971), "Parameter estimates are usually found by repeatedly solving the equations, while varying the parameter estimates to obtain the best fit to size-time data." Size-time data refers to the time series of measured outputs of the system.

These estimated parameters constitute the description of the constituents or components of the compartment. Application of these descriptive parameters to the same compartment with the same components in a different environment is not necessarily valid. For this type of extrapolation to be valid, the effects of potentials and environmental interactions must be extracted from the descriptive parameters.

Explicit inclusion of potentials in models of environmental systems will allow a more realistic and useful representation of the system by (1) differentiating between potential energy storage, kinetic energy storage, and dissipation within a compartment, (2) explicitly representing the environmental resistance to flow between compartments, and (3) permitting application of the descriptive parameters for a compartment to a model of a different environment. The probability of finding two compartments (e.g., the first trophic levels) in different environmental systems with the same components is low. However, when potentials are included explicitly in the modeling process, the individual species may be modeled as components and the resulting descriptive parameters may be used in any environment.

This report develops the method of component description and illustrates its use in terms of hydraulic flow and oxygen concentrations for sediment-water microcosms. The component description concept is especially useful in providing an operational as well as a more accurate description of the potentials, fluxes, and composition of environmental systems. Understanding of environmental manipulation and management will be more complete if the conceptual understanding and analysis is more complete.

THEORETICAL DEVELOPMENT OF COMPONENT MODELING

Overview and Definitions

Complementary variables, a potential and a related flux, must be included in the conceptual model of the system in order to formulate a component description of the system in the nonempirical (symbolic or mathematical) domain. An acceptable set of complementary variables is available from the fundamental equation of classical thermodynamics

$$(dU = Tds - PdV + e\,dq + Fdx + A_i\,dfi + \ldots) \quad (1)$$

However, classical application of these complementary variables to some of the processes in environmental systems is inadequate due to the non-equilibrium state of these systems. Irreversible thermodynamics provides a powerful tool in the form of cross coupling of potentials and fluxes which allows extension of the use of these complementary variables to the description of environmental systems (Morowitz, 1968; Katalchsky and Curran, 1965).

A set of three basic components is defined for each energy form in the system. These are a resistance which represents an energy dissipation, a capacitance which represents a storage of potential energy, and an inertance which represents a storage of kinetic energy.

In addition to the three basic components which are characteristic of each energy form, there are two connective components and two energy transfer components which are universal with respect to energy. The connective components, the potential junction, and the flux junction describe the energy pathways for the interaction of the components within an energy form. The energy transfer components, the transformer, and the gyrator describe the energy pathways for interaction between components in different energy forms.

When information is transferred with negligible flow of energy (e.g., a virus controlling a cell or a signal controlling a fluid valve), it is necessary to introduce a modulated transfer component or a controlled source, depending upon whether the controlled energy is supplied by the system or the environment.

It is not necessary to assume linear components in the description. In fact, environmental systems exhibit inherently nonlinear behavior (Fox, 1971). Nonlinear components complicate the mathematical manipulation and as stated by Fox (1971), "Currently, a nonlinear theory of non-equilibrium thermodynamic processes does not exist." Consequently, as a first approximation, linear components are assumed. The resulting formulation is valid if the system is not too far removed from equilibrium (Boudart, 1968; DeGroot, 1963; Callen, 1960; Prigogine, 1961). Essential nonlinearities can be introduced after the linear description has been satisfactorily completed.

Symbolism-bond graphs

The initial component description of the system is best formulated in a graphic symbolism. The bond graph representation of Karnopp and Rosenberg (1968) is a good choice for systems in which energy flow and transformation are of primary concern. The nature of the graphic description is dependent upon the investigator's conceptual model of the processes occurring in the system and the degree of resolution desired from the resulting mathematical model. (This is also related to the data which is available or which can be measured from experiment with the system.) The graphical representation is the heart of the component description of the system because the applicability of ensuing analysis is limited by the ability of the investigator to represent his conceptual model of the processes in graphic form.

The graphical representation can be improved by iteration. After application of the analytical techniques any unusual or unexpected component values may be interpreted in terms of modification of the components or connectivity of the original graphical representation.

System equations

After the graphical representation is complete the system equations may be reduced to a standard form by application of state space formulation techniques. The state space formulation has the advantages of a large body of descriptive literature (e.g., Desoer, 1970; Martens and Allen, 1969; DeRusso et al., 1965), wide application, and extension to nonlinear components. The system equations may be reduced to a state space form by algebraic or matrix manipulation (Karnopp and Rosenberg, 1968).

The system transfer function can be derived by algebraic or matrix manipulation from the state space formulation of the system equations. This transfer function, which is defined as the ratio of the Laplace transform of the output variable to that of the input variable, is a function of the component values.

The system transfer function can also be obtained from the experimental measurements of the inputs and outputs. This transfer function is expressed as an infinite series function of the complex or Laplace variable, s (Ba Hli, 1971). By equating coefficients of equal powers of s in the two expressions for the transfer function, the component values can be determined whether they exist as discrete physical entities or not.

The component values and state space formulation constitute a complete component description of the system in the nonempirical domain. The analysis of response, stability, and sensitivity of the system model can be pursued using differential calculus and/or computer simulation techniques which are applicable to systems of first order, linear, differential equations with constant coefficients.

Complementary variables

In approaching any problem, an investigator must first form a mental image or conceptual model of the problem. This conceptual model is not well defined and probably varies considerably from one investigator to another. With the complex problems associated with environmental systems, solving and/or communicating the conceptual model requires translating it into the nonempirical language of mathematics or symbolic logic. The substance of the nonempirical representation is dependent upon the original conceptual model. In order to apply component description and analysis to environmental systems the conceptual model must include complementary variables, potentials, and fluxes.

Complementary variables are a pair of variables which may be related mathematically to describe the energy processing function of a component. The pair consists of a potential and a flux. The potential is referred to as the intensive variable in thermodynamics (Callen, 1960), the transvariable in engineering (MacFarlane, 1964), and the across variable in systems theory (Martens and Allen, 1969). The flux is referred to as the extensive variable in thermodynamics (Callen, 1960), the pervariable in engineering (MacFarlane, 1964), and the through variable in systems theory (Martens and Allen, 1969). The potential must be measured between two points, one of which is a reference and is independent of the amount of material present. The flux may be measured at one point and is dependent upon the amount of material present (i.e., the "size" of the component). It is erroneous to think of the potential and flux as cause and effect since either may be the independent variable in a system (Tribus, 1961).

Engineering and systems theory require that the product of the potential and flux be power (MacFarlane, 1964; Martens and Allen, 1969). Classical thermodynamics requires that it be energy (Callen, 1960). Irreversible thermodynamics requires that the product be either energy (Katchalsky and Curran, 1965) or, more commonly, entropy (Prigogine, 1961; DeGroot, 1963; Callen, 1960). The power product will be used in this discussion so that commonly accepted energy storage components may be defined later.

A conceptual model which is based upon a set of descriptive variables that meet the above requirements for complementary variables may be translated into a component description in the nonempirical, mathematical model. Examples of complementary variables for several forms of energy are presented in Table 1.

Table 1. Complementary variables for several energy forms.

Energy Form	Potential	Flux
Mechanical	Force (F)	Velocity (v)
Hydraulic	Pressure (P)	Volume flow rate (Q)
Pneumatic	Pressure (P)	Weight flow rate (q)
Electrical	Voltage (e)	Current (i)
Chemical	Affinity (A)	Extent of reaction flow rate (f)

The choice of force as the potential and velocity as the flux for the mechanical energy form is not in agreement with the definitions of potential and flux. This choice is made so that the development of the potential energy and kinetic energy storage components will agree with the historical development of mechanical systems. This transposition of mechanical potential and flux causes no difficulty because the treatment of potential and flux is symmetrical in the bond graph description of systems which follows (Karnopp and Rosenberg, 1968).

Classical application of paired complementary variables does not adequately describe some of the energy processes which may occur in environmental systems which are not in the equilibrium state (e.g., streaming potential and active transport). However, application of these variables through the concepts of irreversible thermodynamics can describe many of these phenomena. One of the basic concepts of irreversible thermodynamics is that a potential may be phenomenologically related to any flux in addition to the flux of the same energy form with which it is classically associated (e.g., a temperature gradient may be related to a volume rate of flow; Taylor, 1963). Analogously a flux may be phenomenologically related to any potential (e.g., a volume rate of flow may be related to a voltage gradient). These relationships are referred to as cross coupling of potentials and fluxes; the related phenomena in conceptual models will permit a component description and analysis of most environmental systems.

Description of Components

A component is a mathematical model of a physical process involving energy flow or transformation. The mathematical model relating the complementary variables of potential and flux for a component may be either linear or nonlinear in form. Linear components are used in approximations of nonlinear processes because of the greatly simplified nature of the mathematics and stability of computer simulations of the system behavior. The error due to the linear approximation is not too large if the system state does not vary too far from the state for which the approximation is made and if the state for which the approximation is made is not too far removed from equilibrium (Boudart, 1968; DeGroot, 1963; Callen, 1960; Prigogine, 1961). (In this discussion all symbols for parameters and variables will be defined once but can be referred to in the appendix.)

The resistance, capacitance, and inertance components

The resistance is a component which is used to represent the ratio of potential difference to flow rate in a given medium. The parameter used to describe the property of the resistance component is also called the resistance. This parameter is a measure of the potential difference necessary to move a unit of flow through the component in a unit time. The product of the potential difference and the flux associated with the resistance component is a measure of the power dissipated by the component. The mathematical representation of the linear resistance component is

$$R = E/I \quad . . . . . \quad (2)$$

in which E is a potential, I is a flux, and R is the resistance.

The capacitance is a component which is used to represent the storage of potential energy. The parameter used to describe the property of the capacitance component is also called the capacitance. A water tank which stores hydraulic pressure can be modeled as a fluid capacitance. The mathematical representation of the linear capacitance component is

$$C = I \Big/ \left(\frac{dE}{dt}\right) \quad . . . . . \quad (3)$$

in which C is the capacitance value and t is time.

The inertance is a component which is used to represent the storage of kinetic energy. The parameter used to describe the property of the inertance component is also called the inertance. The energy of flow which is stored in the inertia of the mass of fluid moving through a pipe can be modeled as a fluid inertance. It is this stored energy which gives rise to the water hammer effect when a valve is closed quickly. The mathematical representation of the linear inertance component is

$$L = D \Big/ \left(\frac{dI}{dt}\right) \quad . . . . . \quad (4)$$

in which L is the inertance.

Sources

Sources are components which are used to represent potentials and fluxes which originate outside the defined system boundaries. The potential source provides a potential as defined by a specified function of time. The flux source provides a flux as defined by a specified function of time. Agricultural runoff can be modeled as a chemical potential source in describing an aquatic environment.

Controlled sources are components which are used to represent coupled potentials and fluxes or information transfer. The potential or flux of a controlled source depends upon the value of a specified variable some place in the system. For example, when the flux of a chemical compound depends upon the flux of the fluid in which it is suspended or dissolved, then a controlled chemical flux source, which is dependent upon the flux value in the hydraulic subsystem, can be included in the chemical subsystem. When a signal controls an energy process with negligible power transfer, then a form of information transfer occurs which can be modeled with a controlled source. The effect of a catalyst on a chemical reaction is an example of this type of control.

Transfer components

The transformer and gyrator are transfer components which are used to represent an exchange between kinetic and potential energy within or between energy forms. The power into a transfer component equals the power out but the ratio of potential to flux for the power input differs from the ratio for the power output. For the transformer (TF) the potential in is related to the potential out and the flux in is related to the flux out. The mathematical representation of the ideal, linear transformer component is

$$E_{in} = n\, E_{out} \quad . . . . . \quad (5)$$

$$I_{in} = 1/n\, I_{out} \quad . . . . . \quad (6)$$

in which n is the transformer ratio.

For the gyrator (GY) the potential in is related to the flux out and the flux in is related to the potential out. The mathematical representation of the ideal linear gyrator component is

$$Ein = m\ Iout \quad \ldots\ldots\ldots\ldots (7)$$

$$Iin = 1/m\ Eout \quad \ldots\ldots\ldots\ldots (8)$$

in which m is the gyrator ratio. A mechanical lever is an example of a gyrator component.

The modulated transformer and modulated gyrator are transfer components in which the transfer ratios (n and m) are functions of specified variables within the system. These components can be used to represent control of energy processes by information transfer.

Connective components

The potential junction and flux junction are connective components which are used to represent the pathways for interaction of components. The mathematical representation of the potential junction is

$$E_1 = E_2 = E_3 \quad \ldots\ldots\ldots (9)$$

$$I_1 + I_2 + I_3 = 0 \quad \ldots\ldots\ldots (10)$$

The mathematical representation of the flux junction is

$$E_1 + E_2 + E_3 = 0 \quad \ldots\ldots\ldots (11)$$

$$I_1 = I_2 = I_3 \quad \ldots\ldots\ldots (12)$$

The potential junction and flux junction represent parallel and series pathways, respectively.

The mathematical description of the three basic components (the resistance, the capacitance, and the inertance) for several energy forms is presented in Table 2.

The chemical components

The mathematical descriptions of the chemical components (resistance and capacitance) in Table 2 are linear approximations for chemical reactions near equilibrium. These approximations are realistic when

$$|\Delta G| < RT \quad \ldots\ldots\ldots (13)$$

(in which G is Gibb's free energy, R is the gas constant, and T is the absolute temperature) and when

$$\left| N_i - \frac{(N_i)e}{N_i} \right| < 1 \quad \ldots\ldots\ldots (14)$$

(in which N_i is the number of moles of compound i and $(N_i)e$ is the number of moles of compound i at equilibrium) (Boudart, 1968).

The mathematical description of the chemical inertance component is not apparent from developments in chemical kinetics. The inertance component represents a process in which kinetic energy is stored. This indicates that in a chemical inertance the rate of change of extent of reaction (reaction rate) will be stored as kinetic energy (i.e., maintained or supported).

Boudart (1968) states that the basic assumption of the transition state theory of chemical kinetics is that if the products are instantaneously removed from the chemical system at equilibrium, the reaction rate in the forward direction is maintained at the exchange rate prevailing at equilibrium. Thus the value of the chemical inertance parameter is related to the concentration of the activated complex in the transition state. This concentration is in turn a function of the transition frequency along the reaction coordinate and the partition functions for degrees of freedom of translation, rotation, vibration, and interaction of the reacting molecules.

The physical resolution required for application of the preceding concepts from quantum chemistry is much greater than the degree of resolution with which environmental systems are normally defined. Possibly, empirical estimations of the chemical inertance parameter for specific reactions can be determined when indicated by the conceptual model of the system. In this case, the mathematical representation of the chemical inertance is

$$A = L_c \frac{df}{dt} \quad \ldots\ldots\ldots (15)$$

in which L_c is the chemical inertance parameter.

System Graphics

Direct translation of the conceptual model of the system into a mathematical representation is awkward and difficult. It is best to represent the conceptual model in some form of graphic symbolism before proceeding to the mathematical representation.

Circuit diagrams (Close, 1963), compartment diagrams (Odum, 1971), block diagrams (Kuo, 1962), signal flow graphs (Kuo, 1962), linear graphs (Martens and Allen, 1969), and bond graphs (Karnopp and Rosenberg, 1968) are all examples of graphic representation of systems. Each has advantages and disadvantages depending upon the nature of the system to be described. The bond graphs of Karnopp and Rosenberg (1968) are excellent symbolic representations for component description of environmental systems where energy flow is an important process. Following is a summary of the development of bond graphs from "Analysis and Simulation of Multiport Systems" by Karnopp and Rosenberg (1968).

Table 2. Mathematical description of the basic components for several energy forms.

Energy Form	Resistance (R)	Capacitance (C)	Inertance (L)
Mechanical	$F = Bv$	$v = k^{-1}\, dF/dt$	$F = m\, dv/dt$
Hydraulic	$P = (\frac{128\mu l}{d^4})Q$	$Q = (\frac{A_r}{\rho g})dP/dt$	$P = (\frac{\rho l}{A_r})\, dQ/dt$
Pneumatic	$P = R_p q$	$q = (\frac{V}{\beta})\, dP/dt$	$P = (\frac{\rho_o l}{A_r})\, dq/dt$
Electrical	$e = R_e i$	$i = C_e de/dt$	$e = L_e di/dt$
Chemical	$A = (\frac{RT}{Vr})f$	$f = \frac{1}{RT\nu}\, dA/dt$	(see text)

Notation

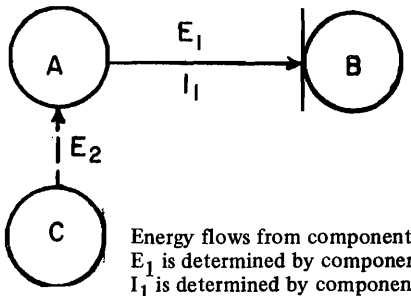
A	=	chemical affinity	Q	=	volume flow rate
A_r	=	area	q	=	weight flow rate
B	=	coefficient of viscous friction	R	=	gas constant
C_e	=	electrical capacitance	R_e	=	electrical resistance
d	=	diameter	R_p	=	pneumatic resistance
e	=	electrical potential	r	=	equilibrium exchange rate
F	=	force	T	=	absolute temperature
f	=	extent of reaction rate	t	=	time
g	=	acceleration due to gravity	v	=	velocity
i	=	electrical current	V	=	volume
k	=	spring constant		=	viscosity
L_e	=	electrical inductance		=	stoichiometric coefficient
l	=	length		=	density
m	=	mass	o	=	average density
P	=	pressure			

In the bond graph representation of a system (refer to Figure 1), a line segment is called a bond and represents a pathway for energy interaction of components. A dotted line segment, called an active bond, represents a pathway for information transfer.

The components are represented by circles with a mnemonic identification inside. The potential associated with a particular pathway (bond) is indicated symbolically above or on the left of the line segment. The associated flux is indicated symbolically below or to the right. An arrow on the bond indicates the direction of positive energy flow (or control for the active bond).

The causal stroke, a bar on the end of a line segment, indicates that a flux on that bond is defined by the component nearest the causal stroke and the potential by the component farthest from the causal stroke. The causal stroke defines the independent and dependent variables for each component. Bond graph representation of the components is summarized in Table 3.

Graphical representation of the conceptual system model is the most important single step in the analysis of system behavior. The system equations which will be solved to determine system behavior, stability, and sensitivity are derived explicitly from the graphical

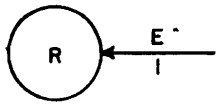
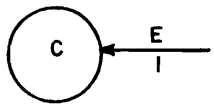
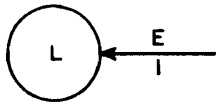
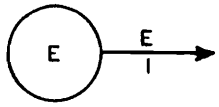
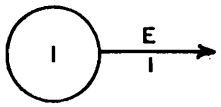
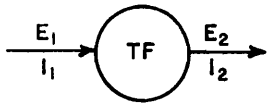
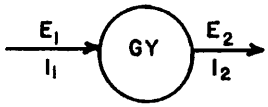
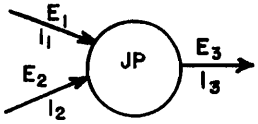
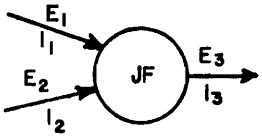


Energy flows from component A to B
E_1 is determined by component A
I_1 is determined by component B
I_2 in component C controls component A's function

Figure 1. Bond graph symbolism.

representation. Decomposition of the real world into a set of interconnected components is a trial and error process based upon the investigator's conceptual model of the physical reality and the intended use of the resulting system representation. There is no best or correct graphical representation of a system, only degrees of realism.

Table 3. Component bond graphs and mathematical representations.

Component	Bond Graph	Mathematical Representation
Resistance		$E = RI$
Capacitance		$I = C\ dE/dt$
Inertance		$E = L\ dI/dt$
Potential Source		$E_1 = E(t)$
Flux Source		$I_1 = I(t)$
Transformer		$E_1 = nE_2$ $I_1 = (1/n)I_2$
Gyrator		$E_1 = mI_2$ $I_1 = (1/m)E_2$
Potential Junction		$E_1 = E_2 = E_3$ $I_1 + I_2 + I_3 = 0$
Flux Junction		$E_1 + E_2 + E_3 = 0$ $I_1 = I_2 = I_3$

Mathematical Analysis of Bond Graph Representation

State space equations

> The state of a system is (defined by) the set of variables, the state variables, which contain sufficient information about the present condition of the system to permit the determination of all future time history of the system, provided that all future inputs are known (Martens and Allen, 1969, p. 71).

Although the quote implies that the system must be studied in a deterministic fashion, this is not necessarily true. Stochastic inputs and functions which are time variant or invariant can be utilized to develop rational models of systems with random variations.

The potential variables on the potential energy storage components and the flux variables on the kinetic energy storage components usually constitute a sufficient set of state variables (Martens and Allen, 1969). The state variables define the system's "memory." In other words, the state variables are sufficient to describe the energy available in the system which may affect system behavior.

After the system has been represented in bond graph form, a systematic technique may be used to derive the system equations in a standard form. The standard form for state space equations is

$$\frac{d}{dt}[X] = [A][X] + [B][U]$$

$$[Y] = [C][X] + [D][U] \quad \ldots\ldots (16)$$

in which the brackets indicate matrices, X is a state variable, U is an input, Y is an output, and A, B, C, and D are coefficients.

The first step in systematic reduction of the bond graph to the state space equations is to name the bonds. A numerical subscript on the pair of variables on each bond serves to identify each component and variable.

The next step is to assign causality to each bond in the graph. This defines the independent variable in each of the component equations. The following steps are used to assign causality to the bonds in the graph.

1. The potential on the bond of a potential source is an independent variable. The potential on this bond is defined or "caused" by the potential source.
2. The flux on the bond of a flux source is an independent variable.
3. The potential on the bond of a capacitance is an independent variable.
4. The flux on the bond of an inertance is an independent variable.
5. The independent variables determined by steps 1 through 4 are used in the equations for the connective components (Equations 9 through 12) to define the independent variables on the connective component bonds.
6. The independent variables on the bonds of the resistances are chosen so that all bonds have a causal stroke which defines the independent variables.

Conflicts in causal assignment may indicate an unrealistic graphical representation of the physical situation.

At this stage the component equations may be transcribed and algebraically manipulated to the standard state space form (Equation 16). However, for large systems (greater than three storage components) the algebra becomes awkward and the matrix reduction which follows is recommended.

To continue the systematic reduction, the bond graph variables are divided into five classes. The state variables (X) are the potentials on capacitances and the fluxes on inertances. The input variables (U) are the potentials on potential sources and the fluxes on flux sources. The temporary variables (T) are the independent variables on the resistances. The auxiliary variables (H) are the independent variables on the transfer components (TF and GY) and the connective components (JP and JF). The output variables (Y) are chosen by the investigator for descriptive purposes.

The relations for a system of linear components may be written in matrix form as

$$\frac{d}{dt}[X] = [C_{11}][X] + [C_{12}][T] + [C_{13}][H] + [C_{14}][U]$$

$$[T] = [C_{21}][X] + [C_{22}][T] + [C_{23}][H] + [C_{24}][U]$$

$$[H] = [C_{31}][X] + [C_{32}][T] + [C_{33}][H] + [C_{34}][U]$$

$$\ldots\ldots\ldots (17)$$

Equation 17 may be reduced to standard state space form in the following manner:

$$[H] = ([I_d] - [C_{33}])^{-1}([C_{33}][X] + [C_{32}][T] + [C_{34}][U])$$

$$[H] = [C'_{31}][X] + [C_{32}][T] + [C'_{34}][U]$$

$$[T] = \{[I_d] - ([C_{22}] + [C_{23}][C'_{32}])\}^{-1}\{([C_{21}] + [C_{23}][C'_{31}])[X] + ([C_{24}] + [C_{23}][C'_{34}])[U]\}$$

$$[T] = [C'_{21}][X] + [C'_{24}][U]$$

$$\frac{d}{dt}[X] = ([C_{11}] + [C_{12}][C'_{21}] + [C_{13}][C'_{31}] + [C_{13}][C'_{32}][C'_{21}])[X] + ([C_{14}] + [C_{12}][C'_{24}] + [C_{13}][C'_{34}] + [C_{13}][C'_{32}][C'_{21}])[U]$$

$$\frac{d}{dt}[X] = [C''_{11}][X] + [C''_{14}][U]$$

$$\ldots\ldots\ldots (18)$$

Equation 18 is of the same form as the standard state space Equation 16 in which [A] = $[C''_{11}]$ and [B] = $[C''_{14}]$.

System transfer functions

The system function or transfer function [H(s)] is defined for a system without time varying coefficients as the ratio of the Laplace transform of the output to the Laplace transform of the input when there is no initial stored energy (DeRusso et al., 1965).

$$H(s) = Y(s)/U(s) \quad \ldots\ldots\ldots\ldots (19)$$

A time varying transfer function [H(t,s)] may be found for systems with time varying coefficients (DeRusso et al., 1965). A matrix transfer function [H(s)] may be determined for systems with more than one input and/or output (Ogata, 1967).

It is useful in the analysis of environmental systems to amend the definition of the transfer function to allow nonzero values of initial stored energy, since some environmental systems cease to function when internal energy equals zero. In this case the observed transfer function $[H^*_{ab}(s)]$ between output a and input b becomes

$$H^*_{ab}(s) = [C_{aj}](s[I_d] - [A])^{-1}[B_{jb}] + [D_{ab}] + \{[C_{aj}](s[I_d] - [A])^{-1}[X(0)]\}/[U_b(s)] \quad \ldots\ldots\ldots (20)$$

in which [A], [B], [C], and [D] are the coefficient matrices of the state equations, $[I_d]$ is the identify matrix, j is the number of state variables, [X(0)] is the initial value vector, and s is the complex frequency or Laplace variable. The observable transfer function of the system for a given input may be obtained from the bond graph through the system equations by application of Equation 20.

The observable transfer function may also be determined from the input and output data which are obtained from system measurements (Ba Hli, 1971). If the input is expresssed as a time series ($\{U_1, U_2, U_3, \ldots\} = \{U\}$) and the output is expressed as a time series ($\{Y_1, Y_2, Y_3, \ldots\} = \{Y\}$), then the time series of areas under the impulse response curve $\{h_a\}$ can be found by synthetic division of the output time series by the input time series as shown in Figure 2.

The observable transfer function H*(s) may be determined from $\{h_a\}$ by

$$H^*(s) = \sum_1^n h_{an} - s \Sigma h_{an} t_n + \frac{s^2}{21} \Sigma h_{an} t_n^2 - \ldots \quad \ldots\ldots\ldots (21)$$

$$U_1, U_2, U_3, \ldots \quad \frac{h_{a1}, h_{a2}, h_{a3} \cdots h_{an}}{Y_1, Y_2, Y_3, \cdots U_n}$$

$$\underline{a_1, a_2, a_3, \cdots a_n}$$
$$b_2, b_3, \cdots b_n$$

$$\underline{c_2, c_3, \cdots c_n}$$

Figure 2. Synthetic division.

in which s is the complex frequency or Laplace variable, h_{an} is the value of h_a in the n^{th} time interval, and t_n is the time value at the middle of the n^{th} time interval.

Component Analysis

Some of the energy processes in environmental systems which may be modeled as components are not physically discrete entities. The chemical resistance component in a representation of the processing of oxygen by a species of algae cannot be placed on a table and subjected to varying oxygen affinities to determine the value of its resistance parameter. However, values of some of the components may be found by using the observable transfer function [H*(s)].

The observable transfer function is expressed as a function of component values by Equation 20. It is also expressed as a function of the input-output data by Equation 21. By equating the coefficients of like powers of s in these two expressions, j + 1 independent equations may be generated where j is the number of state variables. These equations may generally be solved for j + 1 unknown component values.

The component values other than the j + 1 accounted for above must be found by other means. Some component values may be easily measured in the physical system and others by specially designed experiments. If the system exhibits a steady state, it is possible in some cases to determine additional component values by setting the derivatives in the state equations to zero (see Component Description and Analysis section for an example).

System Analysis

The state space equations and component values constitute an operational description of the environmental system within the limits imposed by the assumptions and approximations which are made. This mathematical description or model may be used with analytical or simulation techniques to approximate the response of the physical system to modified inputs, damaged components,

and other phenomena. It is certainly more reasonable to use a mathematical model to investigate approximate responses to environmental changes than to wait and see what actually happens to the environment when it is perturbed, e.g., by pollution.

In addition to mimicing the physical system behavior, the state equation model may be used to evaluate properties of the system as a whole (emergent properties). These mathematically derived properties are related to the energy processing and control structure of the system. These properties would be difficult, if not impossible, to determine by experiment on environmental systems, which cannot generally be stopped and restarted in a specified initial state. These total system properties are considered in the context of general system theory (Bertalanffy, 1968).

Properties

The property of stability is a measure of the "boundedness" of the system response as time approaches infinity (DeRusso et al., 1965). In other words, does the system approach a steady state? The property of controllability is a measure of the degree to which the state or output of the system may be modified by inputs to produce a specified state or output within a finite time (Ogata, 1967). The property of observability is a measure of the degree to which the state of the system may be determined from a knowledge of the output over a finite time interval (Ogata, 1967). The property of optimality is a measure of how well a system meets a defined performance index (DeRusso et al., 1965). The stability, controllability, observability, and optimality of linear, time varying, and nonlinear systems is treated extensively in the system analysis literature.

The property of sensitivity is a measure of the state or output change resulting from a parameter perturbation. Sensitivity to a state perturbation from outside the system may also be postulated. Sensitivity measures may also be used to evaluate system response to inherent errors in parameter or initial state determination (Astor et al., 1972). There is a possibility that in highly connected environmental systems the sensitivity along energy processing pathways may be reciprocally related to the sensitivity along information transferring pathways (Patten, 1972). Sensitivity analysis of environmental systems is relatively new and may provide some valuable general statements concerning information and energy in environmental control processes.

The property of independence or summativity is a measure of the degree to which total system response is independent of component interaction (Bertalanffy, 1968). A related property, centralization or individualization, is a measure of the degree to which total system response is dependent upon a single component or group of components (Bertalanffy, 1968). These two total system properties may become important in describing the evolution of environmental systems; however, their current usage appears to be more philosophical than mathematical.

COMPONENT DESCRIPTION AND ANALYSIS OF A HYDRAULIC SUBSYSTEM IN AN AQUATIC MICROCOSM

System Description

The hydraulic subsystem of aquatic microcosms provide an example of how to apply component description and analysis to the total system. The microcosms consist of lucite cylinders approximately 75 cm. high and 14 cm. in diameter which are filled with water to within 2.3 cm. of the top. During the course of the experiment, the input to the hydraulic subsystem was a 0.900 liter pulse of water each 24 hours. In this development it is assumed that the input flow is continuous over the 24-hour period. (The microcosms are described in more detail in the next section.)

The pictorial diagram (Figure 3) indicates the input reservoir, inlet, outlet, and gas trap of the microcosms along with pertinent system variables where P is pressure and Q is volume flow rate. Three separate representations of the system described in Figure 3, a block diagram, schematic circuit diagram, and bond graph, are presented in Figure 4. In the circuit diagram and the bond graph, R_2 is the hydraulic resistance of the input pipe and orifice; C_4 is the hydraulic capacitance of the cylinder; and R_6 is the hydraulic resistance of the output pipe and orifice. The advantages of the energy port components in the bond graph are the single line representation of the energy flow and the explicit representation of the potential and flux.

The flux junction (JF) on the left in the bond graph indicates that the potential source (P_1) and the resistance R_2 have a common flux (i.e., they are in series connection). The potential junction (JP) in the bond graph indicates that the combination of P_1, R_2, and JF has a common potential with the capacitance C_4 (i.e., they are in parallel connection). Finally, the flux junction (JF) on the right indicates that the combination of the preceding components has a common flux with resistance R_6 and the output Q_7 (i.e., they are in series).

The following component equations (see Table 3) may be written for the bond graph. For the potential source (P_1),

$$P_1 = f(t) = \text{input} \quad \ldots\ldots\ldots\ldots (22)$$

For the flux junction (JF) on the left,

$$P_1 - P_2 - P_3 = 0 \quad \ldots\ldots\ldots\ldots (23)$$

$$Q_1 = Q_2 = Q_3 \quad \ldots\ldots\ldots\ldots (24)$$

in which power flow into the junction is defined as positive. For the resistance R_2,

$$P_2 = R_2 Q_2 \quad \ldots\ldots\ldots\ldots (25)$$

For the potential junction (JP),

$$P_3 = P_4 = P_5 \quad \ldots\ldots\ldots\ldots (26)$$

$$Q_3 - Q_4 - Q_5 = 0 \quad \ldots\ldots\ldots\ldots (27)$$

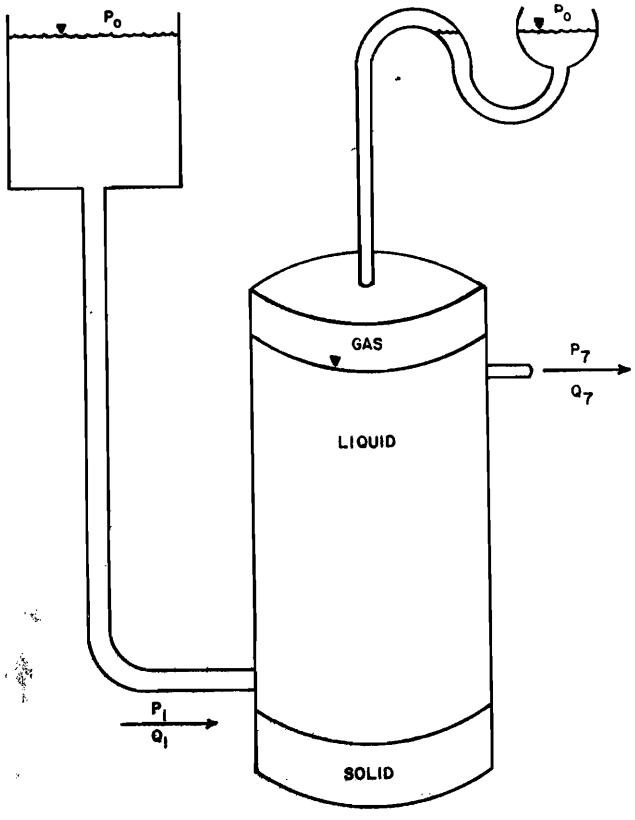


Figure 3. Pictorial diagram of the aquatic microcosm.

For the capacitance C_4,

$$Q_4 = C_4\dot{P}_4 \quad \ldots\ldots\ldots\ldots \quad (28)$$

in which the dot above the P indicates differentiation with respect to time. For the flux junction (JF) on the right

$$P_5 - P_6 - P_7 = 0 \quad \ldots\ldots\ldots\ldots \quad (29)$$

$$Q_5 = Q_6 = Q_7 \quad \ldots\ldots\ldots\ldots \quad (30)$$

For the resistance R_6,

$$P_6 = R_6Q_6 \quad \ldots\ldots\ldots\ldots \quad (31)$$

For the output,

$$Q_7 = \text{output} \quad \ldots\ldots\ldots\ldots \quad (32)$$

$$P_7 = 0 = \text{atmospheric pressure} \quad \ldots\ldots \quad (33)$$

The preceding constitutes the description of the system pursuant to component and state analysis.

State Space Equations

The state variables of the system constitute the system's "memory." These variables are typically the potential on a potential energy storage component and

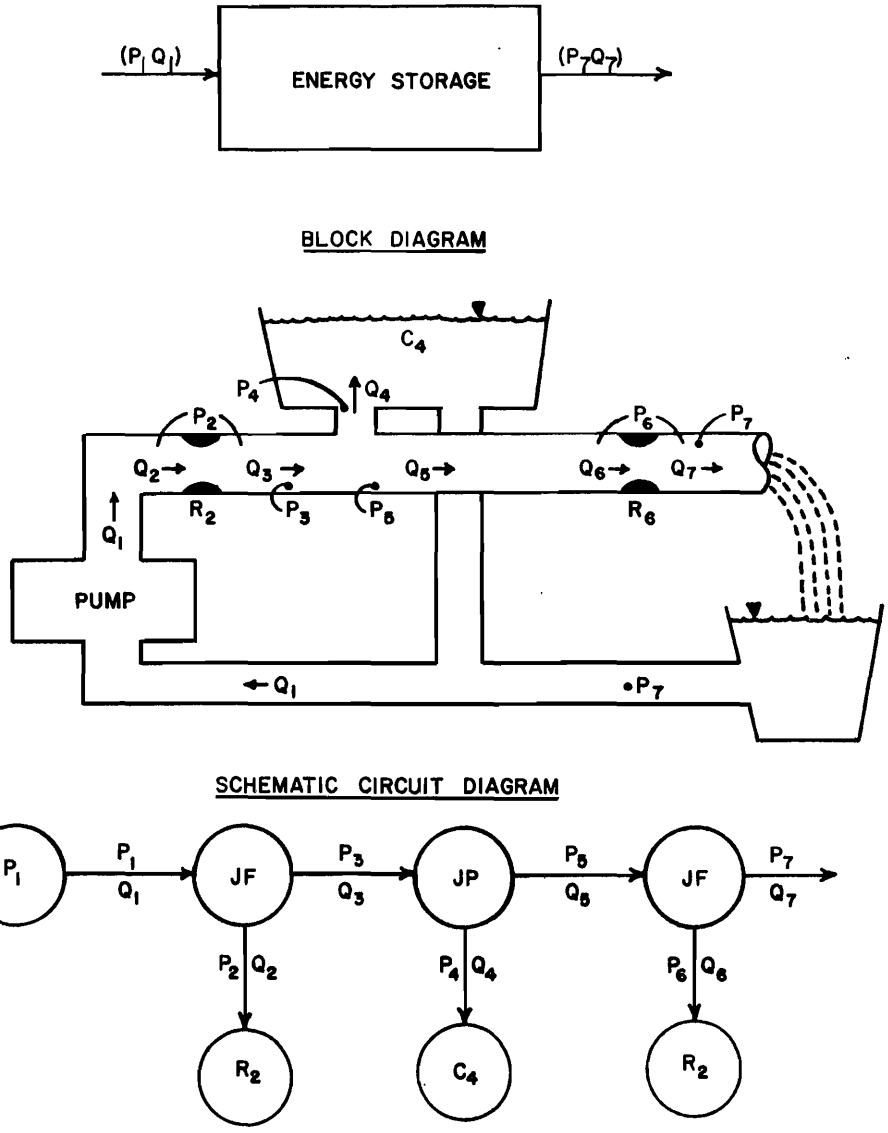


Figure 4. Block diagram, schematic circuit diagram, and bond graph of the aquatic microcosm hydraulic subsystem.

the flux on a kinetic energy storage component. The fluid capacitance (C_4) is the only storage component in the representation of the hydraulic subsystem and the pressure (P_4) is chosen as the state variable because it represents a measure of the potential energy (head) stored in the system.

The component equations (Equations 22 through 33) may be reduced to the standard state space form of Equation 15 by algebraic manipulation. First, combining Equation 23 and Equation 25 gives:

$$P_1 - P_3 = R_2 Q_2 \quad \ldots\ldots\ldots\ldots (34)$$

then substituting from Equation 24 for Q_2 and combining Equation 34 with Equation 27,

$$P_1 - P_4 = R_2 Q_4 + R_2 Q_5 \quad \ldots\ldots\ldots (35)$$

substituting from Equation 30 for Q_5 and combining Equation 35 with Equation 31,

$$P_1 - P_4 = R_2 Q_4 + R_2 R_6^{-1} P_6 \quad \ldots\ldots\ldots (36)$$

solving Equation 29 for P_6 and combining with Equation 33,

$$P_6 = P_5 \quad \ldots\ldots\ldots\ldots\ldots (37)$$

substituting from Equation 26 for P_5 and eliminating P_6 from Equation 36 and Equation 37,

$$P_1 - P_4 = R_2 Q_4 = R_2 R_6^{-1} P_4 \quad \ldots\ldots\ldots (38)$$

substituting from Equation 28 for Q_4,

$$P_1 - P_4 = R_2 C_4 \dot{P}_4 + R_2 R_6^{-1} P_4 \quad \ldots\ldots\ldots (39)$$

finally, solving Equation 39 for $\dot{P}_4$,

$$\dot{P}_4 = (-R_2^{-1} C_4^{-1} - R_6^{-1} C_4^{-1}) P_4 + R_2^{-1} C_4^{-1} P_1 \quad \ldots\ldots\ldots (40)$$

which is the first equation of Equation 15. The second, the output equation, is found by solving the component equations for Q_7, the output, in terms of P_4, the state variable. This is done by substituting for Q_6 in Equation 31 from Equation 30 and solving for Q_7,

$$Q_7 = R_6^{-1} P_6 \quad \ldots\ldots\ldots\ldots (41)$$

then substituting from Equation 37 for P_6 and from Equation 26 for P_5,

$$Q_7 = R_6^{-1} P_4 \quad \ldots\ldots\ldots\ldots (42)$$

which is the final state space equation.

Matrix reduction

The preceding algebraic reduction of the component equations to standard form is somewhat tedious even for this system of seven components. The matrix reduction equations (Equations 17 and 18) are preferable if a computer is available for the matrix inversion. To write the component equations in a form which is directly amenable to translation to the form of Equation 16, causality must be assigned to the bond graph bonds.

The steps which are used to produce the causal bond graph of Figure 5 are as follows:

1. The potential on the input bond is defined by the potential source (P_1)
2. The potential on the output bond is defined by the atmospheric or reference potential (P_7)
3. The potential on the bond to the capacitor is defined by the state variable (P_4)
4. The remaining two bonds on the potential junction (JP) have their potential determined by the definition of the component
5. Since all but one of the potentials of both of the flux junctions (JF) are defined, the remaining potential is defined by the equation for the flux junction component. Thus the flux on these two remaining bonds is determined by the resistances (R_2 and R_4)

These independent variables in Figure 5 may be propagated through the graph by application of the connective component (JP and JF) equations (Table 3). For example, Q_2 may be extended to the input bond because all fluxes on a flux junction are equal ($I_1 = I_2 = I_3$). The resulting completely causal bond graph is shown in Figure 6 where the extended independent variables are placed in parentheses.

The component equations resulting from the completed causal bond graph in Figure 6 are:

$$\dot{P}_4 = C_4^{-1} (Q_2 - Q_6) \quad \ldots\ldots\ldots\ldots (43)$$

$$Q_2 = R_2^{-1} (P_1 - P_4) \quad \ldots\ldots\ldots\ldots (44)$$

$$Q_6 = R_6^{-1} (P_4 - P_7) \quad \ldots\ldots\ldots\ldots (45)$$

These component equations may easily be written in the matrix form of Equation 16 where the state variable (X) is P_4, the temporary variables (T) are Q_2 and Q_6, and the auxiliary variables (H) are zero because there are no transfer components in the hydraulic subsystem. Thus the matrix form of the component equations (with $P_7 = 0$) is

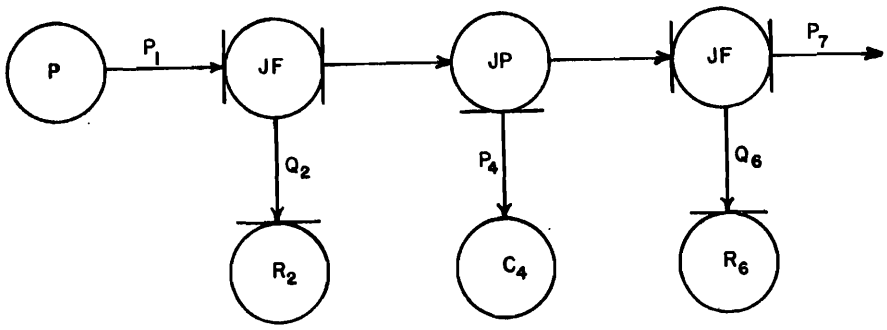


Figure 5. Causal bond graph.

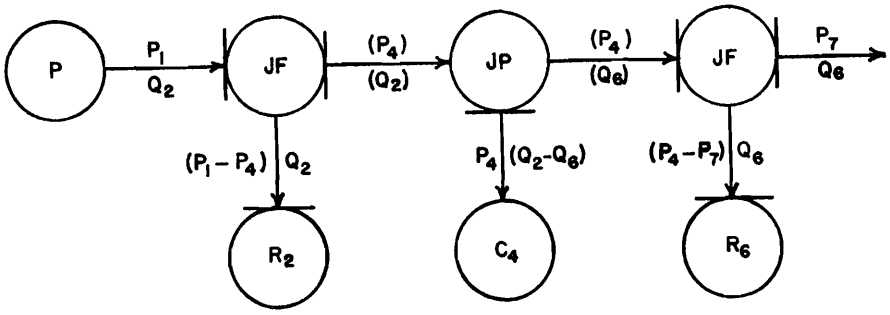


Figure 6. Causal bond graph with completely extended causality.

$$[P_4] = [0][P_4] + [C_4^{-1}, -C_4^{-1}]\begin{bmatrix} Q_2 \\ Q_6 \end{bmatrix} + [0][P_1]$$

$$\begin{bmatrix} Q_2 \\ Q_6 \end{bmatrix} = \begin{bmatrix} R_2^{-1} \\ R_6^{-1} \end{bmatrix}[P_4] + \begin{bmatrix} 0,0 \\ 0,0 \end{bmatrix}\begin{bmatrix} Q_2 \\ Q_6 \end{bmatrix} + \begin{bmatrix} -R_2^{-1} \\ 0 \end{bmatrix}[P_1] \quad \ldots\ldots\ldots\ldots (46)$$

By comparison of Equation 46 with Equation 17, the values of the coefficients C_{ij} may be determined and used in Equation 17 to give

$$[\dot{P}_4] = \left\{[0] + [C_4^{-1}, -C_4^{-1}]\left([I_d] - \begin{bmatrix} 0,0 \\ 0,0 \end{bmatrix}\right)^{-1}\begin{bmatrix} R_2^{-1} \\ R_6^{-1} \end{bmatrix}\right\}[P_4]$$

$$+ \left\{[0] + [C_4^{-1}, -C_4^{-1}]\left([I_d] - \begin{bmatrix} 0,0 \\ 0,0 \end{bmatrix}\right)^{-1}\begin{bmatrix} -R^{-1} \\ 0 \end{bmatrix}\right\}[P_1] \quad \ldots\ldots\ldots\ldots (47)$$

Equation 47 may be simplified by performing the indicated operations which result with

$$\dot{P}_4 = (-R_2^{-1} C_4^{-1} - R_6^{-1} C_4^{-1}) P_4 + R_2^{-1} C_4^{-1} P_1 \quad (48)$$

as the final form for the first of the state equations (Equation 16). The second equation, the output equation, which relates the output (Q_7) to the input (P_1) and state variable (P_4) can be found from Equation 45 and by noting that the completed causal bond graph shows that $Q_7 = Q_6$. The output equation is

$$Q_7 = R_6^{-1} P_4 \quad \ldots\ldots\ldots\ldots (49)$$

The state equations which result from the matrix reduction are identical to those which result from the algebraic reduction (Equations 40 and 42). This set of state space system equations may be used for analysis of system behavior and properties and to determine a system transfer function.

System Transfer Function

The transfer function [H(s)] of the system is defined in Equation 19 for the case when the initial state

of the system is zero as is assumed for the microcosm. An expression for this transfer function may be determined by substituting from the state equations (Equations 48 and 49) into Equation 20 with [X(0)] equal to zero.

$$H(s) = \frac{Q_7(s)}{P_1(s)} = R_6^{-1}(s[1]+R_2^{-1}C_4^{-1} + R_6^{-1}C_4^{-1})^{-1}(R_2^{-1}C_4^{-1}) \quad \ldots\ldots(50)$$

Equation 50 may be rearranged to the more conventional form of

$$H(s) = (R_2^{-1}R_6^{-1}C_4^{-1}) \left[\frac{1}{s+\left(\frac{R_2+R_6}{R_2R_6C_4}\right)}\right] \quad \ldots(51)$$

Equation 51 is of the same form as

$$H(s) = A\frac{1}{s-a} \quad \ldots\ldots\ldots\ldots(52)$$

in which

$$A = \frac{1}{R_2R_6C_4} \quad \ldots\ldots\ldots\ldots(53)$$

and

$$a = \frac{-(R_2+R_6)}{R_2R_6C_4} \quad \ldots\ldots\ldots\ldots(54)$$

Another representation may be determined for this transfer function from the input-output data for the system when the initial state is zero. The output data for a constant input pressure (P_1) with the initial state equal to zero is recorded in Table 4 and graphed in Figure 8.

By application of synthetic division (Figure 2) and Equation 21, the transfer function may be determined. The synthetic division of the scaled output by the scaled input is shown in Figure 7. The unscaled result for the time series h_a is presented in Table 4. Using the values of h_a in Equation 21 results in a transfer function,

```
                    6.34,  1.59,  0.81,  0.44,  0.42,  0.41,  0.11,  0.12,  0.09,  0.12,  -0.12,  0.01
1,1,1,1,1,1,1,1,1,1,1,1) 6.34,  7.93,  8.74,  9.18,  9.60, 10.01, 10.12, 10.23, 10.33, 10.45,  10.44, 10.45
                    6.34,  6.34,  6.34,  6.34,  6.34,  6.34,  6.34,  6.34,  6.34,  6.34,   6.34,  6.34
                           1.59,  2.40,  2.84,  3.26,  3.67,  3.78,  3.89,  3.99,  4.11,   4.10,  4.11
                           1.59,  1.59,  1.59,  1.59,  1.59,  1.59,  1.59,  1.59,  1.59,   1.59,  1.59
                                  0.81,  1.25,  1.67,  2.08,  2.19,  2.31,  2.40,  2.52,   2.51,  2.52
                                  0.81,  0.81,  0.81,  0.81,  0.81,  0.81,  0.81,  0.81,   0.81,  0.81
                                         0.44,  0.86,  1.27,  1.38,  1.50,  1.59,  1.71,   1.70,  1.71
                                         0.44,  0.44,  0.44,  0.44,  0.44,  0.44,  0.44,   0.44,  0.44
                                                0.42,  0.83,  0.94,  1.06,  1.15,  1.27,   1.26,  1.27
                                                0.42,  0.42,  0.42,  0.42,  0.42,  0.42,   0.42,  0.42
                                                       0.41,  0.52,  0.64,  0.73,  0.85,   0.84,  0.85
                                                       0.41,  0.41,  0.41,  0.41,  0.41,   0.41,  0.41
                                                              0.11,  0.23,  0.32,  0.44,   0.43,  0.44
                                                              0.11,  0.11,  0.11,  0.11,   0.11,  0.11
                                                                     0.12,  0.21,  0.33,   0.32,  0.33
                                                                     0.12,  0.12,  0.12,   0.12,  0.12
                                                                            0.09,  0.21,   0.20,  0.21
                                                                            0.09,  0.09,   0.09,  0.09
                                                                                   0.12,   0.11,  0.12
                                                                                   0.12,   0.12,  0.12
                                                                                          -0.01,  0.00
                                                                                          -0.01, -0.01
                                                                                                  0.01
                                                                                                  0.01
```

Note: Input is scaled from 45276 gm. cm.$^{-1}$ sec.$^{-2}$ down to 1 gm. cm.$^{-1}$ sec.$^{-2}$ so each term of the quotient must be divided by 45276.0. Likewise each term of the dividend is scaled by 10^3 so each term of the quotient must be multiptied by 10^{-3}.

Figure 7. Synthetic division of scaled output by scaled input.

Table 4. Output data for the hydraulic subsystem.

Time (sec.)x10^{-3}	Q_7 Flow Rate (cm.^{3}sec.$^{-1}$)x10^3	Mid-Interval Time (sec.)x10^{-3}	Synthetic Division Quotient $\{h_a\}$x10^7
15	6.34	7.5	1.400
45	7.93	37.5	.351
75	8.74	67.5	.179
105	9.18	97.5	.097
135	9.60	127.5	.093
165	10.01	157.5	.091
195	10.12	187.5	.024
225	10.23	217.5	.026
255	10.33	247.5	.021
285	10.45	277.5	.026
315	10.44	307.5	-.002
345	10.45	337.5	.002
		$\sum_{n=1}^{12} h_{an} = 2.308 \times 10^{-7}$	
		$\sum_{n=1}^{12} h_{an}t_n = 9.402 \times 10^{-3}$	

$$H(s) = 2.308\,(10^{-7}) - 9.402\,(10^{-3})s \quad . . (55)$$

The two representations of the transfer function, Equations 52 and 54, may be used in analysis of the component values.

Component Analysis

The component values may be determined from the steady state solution of the system equations and the transfer functions. For this system they may also be determined by physical measurements which are made with the component isolated from the rest of the system. The two sets of component values may be compared to evaluate the accuracy of the component analysis. For many environmental systems, the component values may not be determined by direct physical measurements and the capability of the model to mimic system behavior is the only evaluation of the accuracy of the component analysis.

The height of the water in the reservoir above the microcosm is 46.2 cm, thus, the input pressure (P_1) is

$$P_1 = \rho g h_1 = (1)(980)(46.2) \quad . . . . . (56)$$

$$P_1 = 45276.0 \text{ gm. cm.}^{-1} \text{sec.}^{-2} \quad . . . . . (57)$$

in which ρ is density, g is acceleration due to gravity, and h is height of water. When the system is in the steady state ($Q_7 = 10.45 \times 10^{-3}$ cm.^{3} sec.$^{-1}$), then the height of the water above the outlet in the microcosm is 3.5 cm. From this,

$$P_4 \text{ at } (t = \infty) = \rho g h_4 = (1)(980)(3.5) \quad . . (58)$$

$$P_4 \text{ at } (t = \infty) = 3430.0 \text{ gm. cm.}^{-1} \text{sec.}^{-2} \quad . (59)$$

The output (Q_7) as a function of time is presented in Table 4.

The input pressure and steady state values may be used in the component equations (Equations 43 through 45) of the causal bond graph to determine that

$$\dot{P}_4 = 0 = C_4^{-1}(Q_2 - Q_6) \quad . . . . . (60)$$

or

$$\dot{Q}_2 = Q_6 = Q_7 \quad . . . . . (61)$$

then

$$R_2 = (P_1 - P_4)Q_7^{-1} = 4.004 \times 10^6 \text{ gm. cm.}^{-4} \text{sec.}^{-1} \quad . . . . . (62)$$

$$R_6 = (P_4 - 0.0)Q_7^{-1} = 3.282 \times 10^5 \text{ gm. cm.}^{-4} \text{sec.}^{-1} \quad . . . . . (63)$$

The two representations of the transfer function (Equations 52 and 55) may be equated such that

$$A(s-a)^{-1} = 2.308\,(10^{-7}) - 9.402\,(10^{-3})s \quad . (64)$$

Multiplying Equation 64 by (s-a) gives

$$A = -2.308\,(10^{-7})a + 2.308\,(10^{-7})s + 9.402\,(10^{-3})as - 9.402\,(10^{-3})s^2 \quad . . . (65)$$

Equating coefficients of the first power of s gives

$$-9.402\,(10^{-3})a = 2.308\,(10^{-7}) \quad . . . . . (66)$$

Substituting for a from Equation 54 and solving for C_4 results with

$$C_4 = (9.402)(2.308)^{-1}(10^4)(R_2 + R_6)(R_2 R_6)^{-1} \quad . . (67)$$

Finally, substituting for R_2 and R_6 from Equations 62 and 63 indicates that

$$C_4 = 1.342 \times 10^{-1} \text{ gm.}^{-1} \text{ cm.}^4 \text{ sec.}^2 \quad . . (68)$$

When the output resistance (the output orifice and pipe) is subjected to a pressure of 3920.0 dynes per square centimeter, then the flow rate is 1.129×10^{-2} cubic centimeters per second. From this data the value of R_6 is found as

$$R_6 = P Q^{-1} = 3.472 \times 10^5 \text{ gm. cm.}^{-4} \text{ sec.}^{-1} \quad . (69)$$

Similarly, for R_2 when the pressure is 19600.0 dynes per

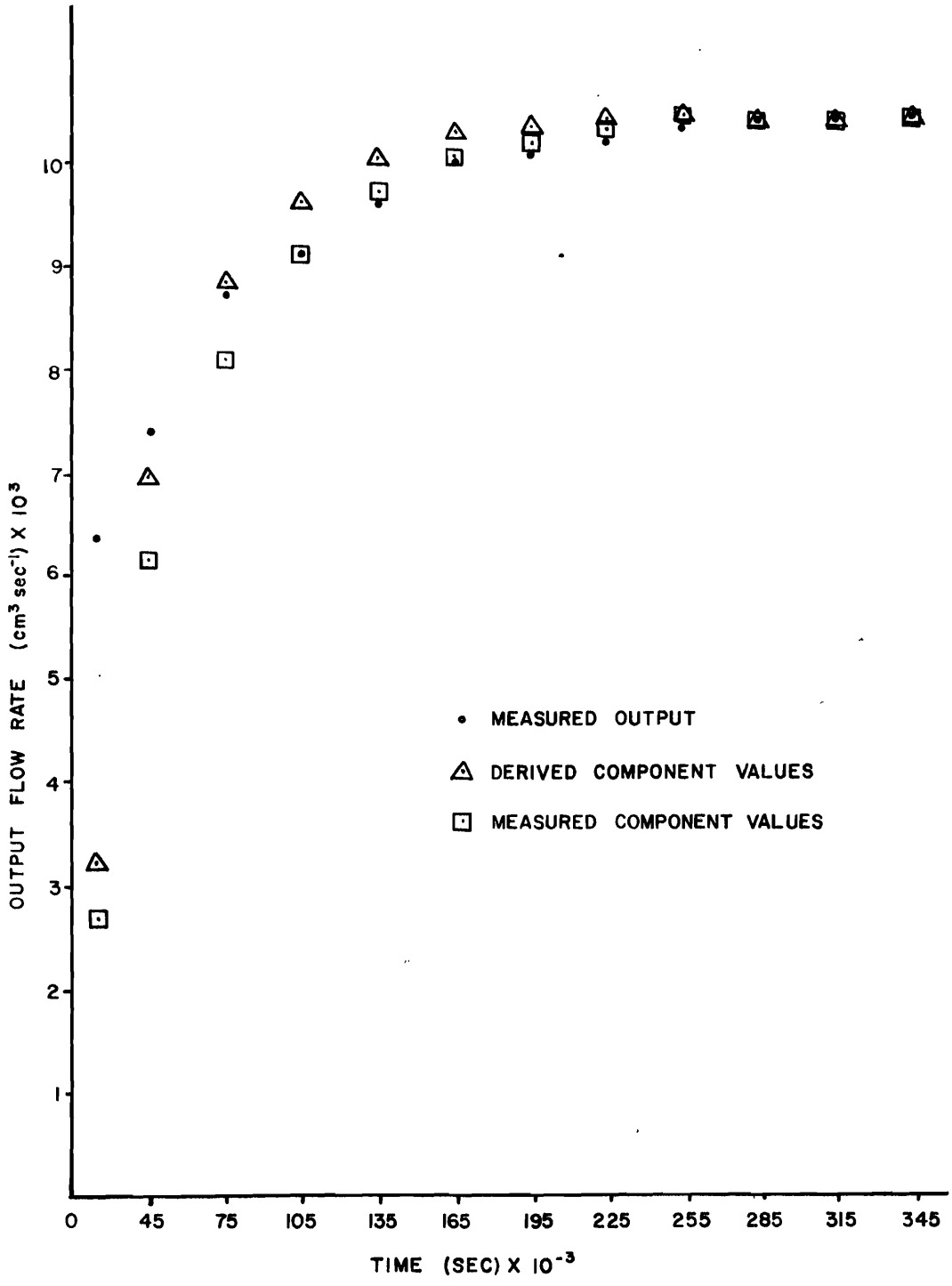


Figure 8. Output of the system and the model.

square centimeter and the flow rate is 4.898×10^{-3} cubic centimeters per second, then the value of R_2 is found from

$$R_2 = PQ^{-1} = 4.001 \times 10^{6}\ \text{gm.}^{-1}\ \text{cm.}^{4}\ \text{sec.}^{2} \quad .(70)$$

The expression for a hydraulic capacitance from Table 4 is

$$C = \frac{A_r}{\rho g}$$

in which A_r is area, ρ is density, and g is acceleration due to gravity. The inside diameter of the microcosm is 14 cm. and thus the capacitance is

$$C = (7)^2 \pi (980)^{-1} = 1.571\ (10^{-1})\ \text{gm.}^{-1}\ \text{cm.}^{4}\ \text{sec.}^{2} \quad . . . . . .(71)$$

As noted earlier, j + 1 (in which j is the number of state variables) variables could be determined from the transfer functions in the absence of physical measurements. The capacitance was determined in this manner in Equation 67. The other equation which might have been used if the steady state data had not been available is found by equating coefficients of s^0 in Equation 65. This equation is

$$A = 02.308\ a \quad . . . . . .(72)$$

Substituting for A and a from Equations 53 and 54 and dividing by $R_2^{-1}R_6^{-1}C_4^{-1}$ gives

$$R_2 + R_6 = (2.308)^{-1}(10^7) = 4.332\,(10^6)\ \text{gm.}^{-1}\text{cm.}^{4}\text{sec.}^{2} \quad . . . . . .(73)$$

which could have been used to determine either R_2 or R_6. The equations for powers of s greater than j + 1 are dependent and provide no additional information.

A comparison of component values found by isolated measurement and those found by component analysis appears in Table 5.

Table 5. Measured and derived component values.

Component	Derived Value	Measured Value	Relative Error
R_2	4.004×10^6	4.001×10^6	0.07%
R_6	3.282×10^5	3.472×10^5	4.2 %
C_4	1.342×10^{-1}	1.571×10^{-1}	14.5 %
$R_2 + R_6$	4.332×10^6	4.348×10^6	0.4 %

System Analysis

The set of state space system equations along with the component values constitutes a complete dynamic description of the system. This set of equations may be solved for the outputs as a function of time by analytical, analog computer, or digital computer techniques.

The set of state space equations for the hydraulic subsystem consists of a state equation (Equation 48) and an output equation (Equation 49). The state equation and output equation may be combined to give a single system equation which is

$$\dot{Q}_7 = (R_2^{-1}C_4^{-1} + R_6^{-1}C_4^{-1})Q_7 + R_2^{-1}R_6^{-1}C_4^{-1}P_1 \quad . . . . . .(74)$$

Equation 74 may be separated and integrated to find the solution

$$\int_0^{Q_7} \frac{dQ}{R_2^{-1}R_6^{-1}C_4^{-1}P_1 + (-R_2^{-1}C_4^{-1} - R_6^{-1}C_4^{-1})Q} = \int_0^t dt \quad . . . . . .(75)$$

Evaluation of the integrals in Equation 75 gives

$$\ln[R_2^{-1}R_6^{-1}C_4^{-1}P_1 + (-R_2^{-1}C_4^{-1} - R_6^{-1}C_4^{-1})Q_7] - \ln(R_2^{-1}R_6^{-1}C_4^{-1}P_1) = (R_2^{-1}C_4^{-1} + R_6^{-1}C_4^{-1})t \quad . . . . . .(76)$$

Solving Equation 76 for Q_7 results in

$$Q_7 = P_1(R_2 + R_6)^{-1}(1 - e^{-(R_2+R_6)R_2^{-1}R_6^{-1}C_4^{-1}t}) \quad . . . . . .(77)$$

Evaluation of the model

Substituting the derived component values from Table 5 into Equation 77 produces

$$Q_7 = 1.045\,(10^{-2})(1 - e^{-2.456(10^{-5})t}) \quad . . .(78)$$

while substituting the measured component values produces

$$Q_7 = 1.044\,(10^{-2})(1 - e^{-1.985(10^{-5})t}) \quad . . .(79)$$

The solutions to Equations 78 and 79 and the measured outputs at specified times are presented in Table 6 and the graph of Figure 8.

It is apparent from Figure 8 that both models mimic observed behavior reasonably well after the time of 75,000 sec. (20 hours and 50 minutes). Prior to this time both models indicate fluxes lower than the observed values.

There are two reasons for the low fluxes prior to 75,000 seconds. First, for low values of P_4 (i.e., low fluid levels in the capacitance C_4) the output orifice and pipe are not filled so that the resistance R_6 is that of an open channel for which

$$P_4 = R_6(P_4)Q_7^2 \quad \ldots\ldots\ldots\ldots (80)$$

The resistance of the outlet for a partially filled circular cross section is a function of the wetted perimeter and area of the flow (Daugherty, 1965); thus, it is a function of P_4 as indicated in Equation 80. Second, even in a situation where the hydraulic resistance is primarily determined by an orifice, the resistance is inherently nonlinear (Shearer et al., 1967) as indicated by

$$P_4[\rho(.5)C_d^{-2}A_r^{-2}]Q_7^2 \quad \ldots\ldots\ldots (81)$$

in which ρ is density, C_d is a discharge coefficient and A_r is the cross sectional area.

If the present models were not satisfactorily accurate for the investigator's purpose, then a piecewise linear resistance or a nonlinear resistance as indicated by Equations 80 and 81 could be included in the models. Additional improvement might include (1) accounting for the storage due to the compliance (i.e., flexibility under pressure) of the input and output pipes, and (2) limiting the maximum value of P_4 since the physical storage capacity is not infinite.

Table 6. Output of the system and the model.

Time (sec) x 10^{-3}=	Measured Output ($cm.^3sec.^{-1}$) x 10^3=	Model Output With Measured Component Values ($cm.^3sec.^{-1}$) x 10^3=	Model Output With Derived Component Values ($cm.^3sec.^{-1}$) x 10^3=
15	6.34	2.69	3.22
45	7.93	6.17	6.99
75	8.74	8.09	8.80
105	9.18	9.15	9.66
135	9.60	9.73	10.07
165	10.01	10.06	10.27
195	10.12	10.23	10.36
225	10.23	10.33	10.41
255	10.33	10.39	10.43
285	10.45	10.42	10.44
315	10.44	10.43	10.45
345	10.45	10.44	10.45

COMPONENT DESCRIPTION AND ANALYSIS OF OXYGEN IN AN AQUATIC MICROCOSM

System Description

The aquatic microcosms (Figure 3) introduced in the preceding section are part of a sediment-water nutrient exchange experiment being conducted at the Utah Water Research Laboratory, Logan, Utah. The sediment samples were taken from Hyrum Reservoir, Utah (see Porcella et al., 1972).

The microcosms consisted of approximately 75 cm. high lucite cylinders which had an inside diameter of 14 cm. They were isolated from the atmosphere by a gas-trap which had a provision for removal of gas samples. The microcosms were filled to a depth of approximately 15 cm. (2.3 liters) with sediments and then with water to a level within 3 cm. of the top seal.

There were 16 microcosms in the experiment arranged in a 4 x 2 x 2 factorial experimental design. The variations of treatments were (1) light (dark, vertical continuous light, horizontal dirunal light of 16 hours, and horizontal light with variable intensity over a diurnal cycle), (2) nitrogen (high and low levels), and (3) mercury (high and low levels). The particular microcosm selected for study in this part is number nine which has vertical continuous light, low nitrogen, and low mercury treatments. This microcosm was selected because it has demonstrated considerable suspended growth of both algae and bacteria and gas production (mostly O_2) compared to the other microcosms.

Each day, 10 percent (about .9 liters) of the volume of water is removed and replaced with fresh nutrient media. Thus the water in the microcosms has a mean residence time of about 10 days.

The water in the microcosms is completely mixed with a water driven magnetic stirrer. They are maintained at a temperature of approximately 25°C.

A complete description of the microcosms, experimental techniques, data, and results can be found in Porcella et al. (1974).

The Bond Graph

The energy processes associated with oxygen in microcosm number nine (henceforth called the microcosm) are to be studied using a component description and analysis of the oxygen subsystem The possible component representations of the oxygen subsystem in the microcosm are innumerable. The representation which follows (Figure 9) is a compromise between simplicity and realism.

In the bond graph of Figure 9, f is a chemical flux (mg per day), A is a chemical potential (Kcal per mg), C is a capacitance for the storage of chemical potential energy, R is a chemical resistance, and TF is a transformer. The component indicated by an arrow is a unilateral flux component. It indicates that flow can only occur in the direction indicated.

The causality and resulting independent variables are indicated on the bonds of the bond graph in Figure 9. The other vairables on the bonds which result from the use of the independent variables in the junction component equations appear in Figure 10.

f_1 is the input of dissolved oxygen in the nutrient media. It is assumed to be a constant value of 7.56 mg per day.

C_3 represents the storage of dissolved oxygen in the water in the body of the microcosm.

R_5 represents the resistance to oxygen exchange between the gas and liquid phases.

C_6 represents the storage of gaseous oxygen in the gas-trap.

R_{10} represents the resistance to the photosynthesis driven breakdown of water to oxygen.

C_{14} represents the storage of oxygen as water.

f_{17} is a controlled flux source which represents the flux of oxygen from dissolved oxygen to the oxygen of water through respiration.

A_{20} is an hypothetical, chemical, potential, source which represents the energy available for the growth of biomass. This source includes the chemical energies of all nutrients and that which results from electromagnetic excitation of the chlorophyll molecules. If one of these

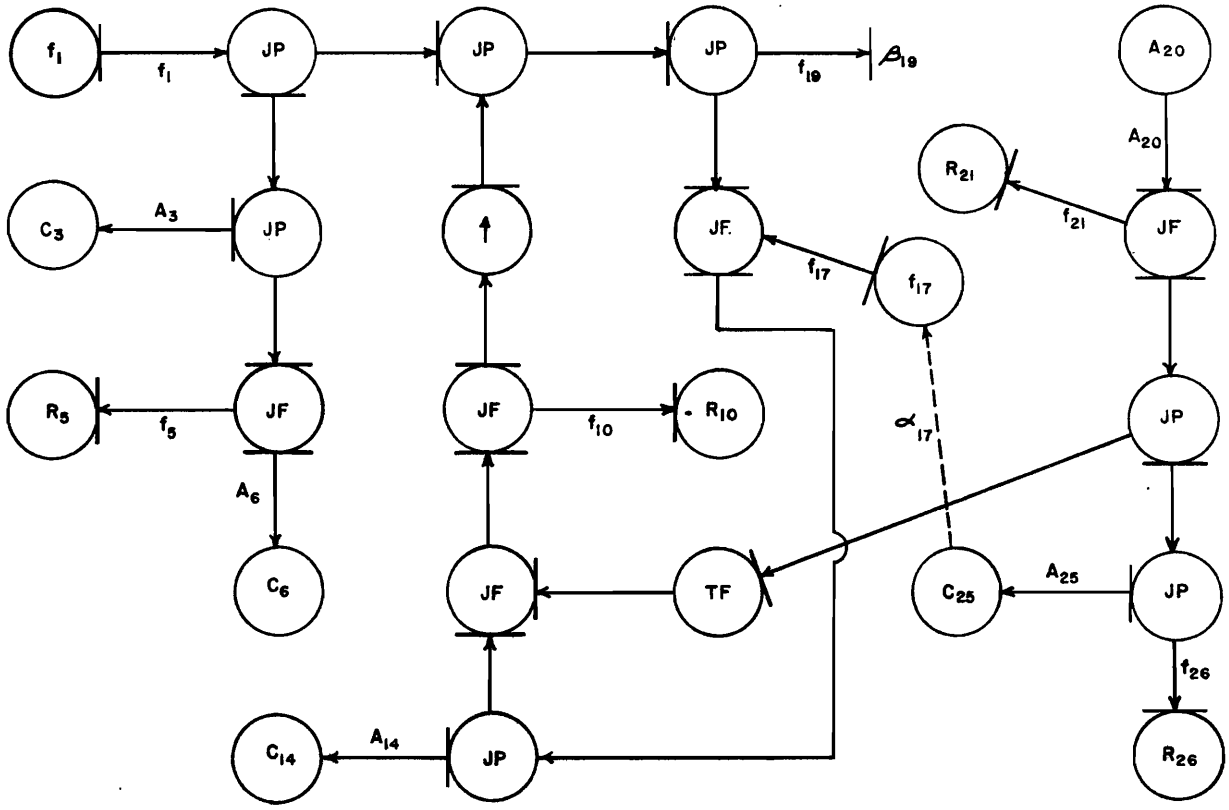


Figure 9. Bond graph of the oxygen subsystem of the microcosm with the independent variables indicated.

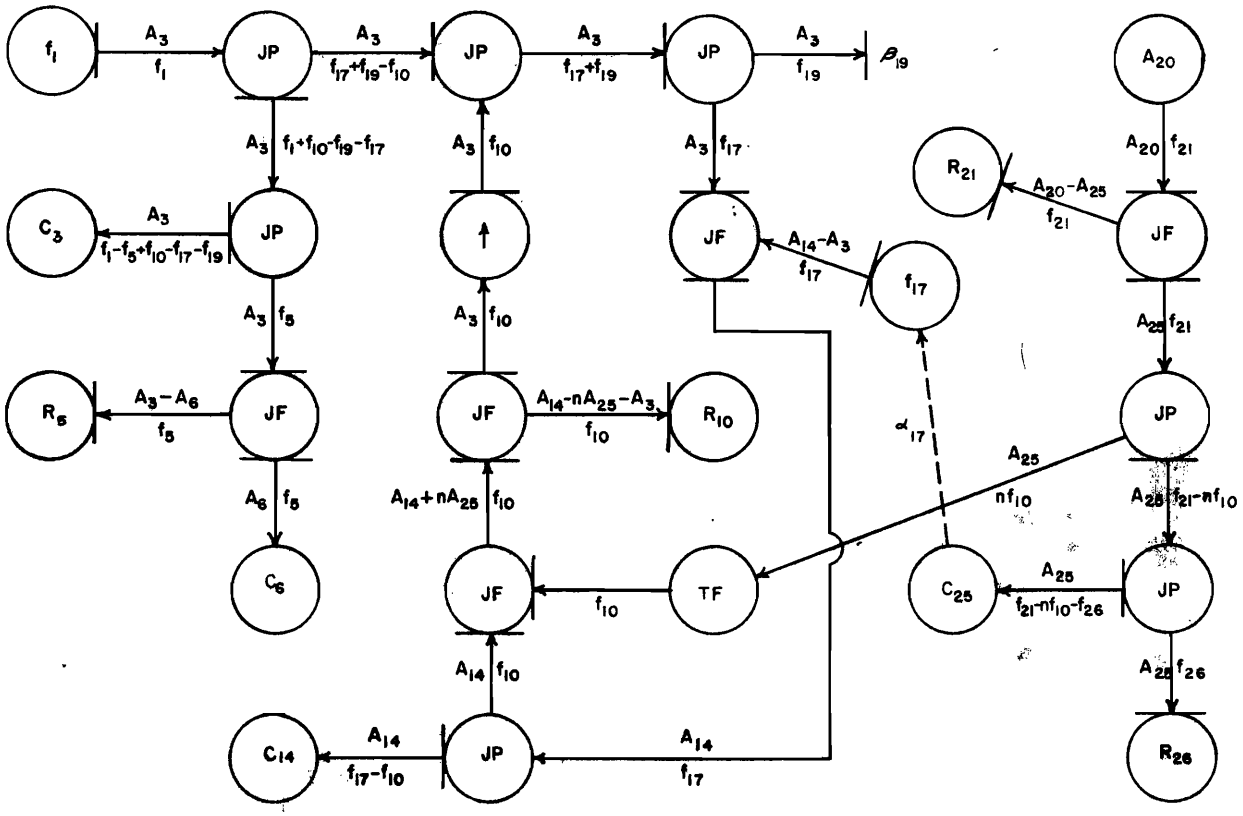


Figure 10. Completed bond graph of the oxygen subsystem.

energy sources were varying considerably and limiting growth, then the energy processing subsystem for that energy source would have to be coupled to the oxygen subsystem to produce a realistic model. In an ideal model A_{20} would be replaced by individual sources and energy processing components for each energy input.

R_{21} represents the growth resistance of the biomass.

C_{25} represents the storage of biomass in the microcosm.

α_{17} is the ratio of the flux, f_{17}, to the potential of the biomass (A_{25}).

β_{19} is the ratio of the flux of oxygen out of the microcosm (f_{19}) to the potential of oxygen in the microcosm (A_3). f_{19} depends on the flux of water out of the microcosm (0.9 liters per day) and the potential (which is proportional to the concentration) of oxygen in the microcosm.

R_{26} represents the decay resistance of the biomass.

TF, the transformer component, represents the use of some of the energy available for photosynthesis to produce oxygen from water.

The Component Equations

The component equations may be written from the bond graph (Figure 10) by using the information in Table 3.

The state variables (X) are A_3, A_6, A_{14}, and A_{25}. The temporary variables (T) are f_5, f_{10}, f_{17}, f_{19}, f_{21}, and f_{26}. There are no auxiliary variables (H) because the potentials and fluxes on the transformer component were written in terms of the state variables, the temporary variables, and the transformer ratio (n). The input variables (U) are f_1 and f_{20}. The output variables (Y) are the same as the state variables.

The component equations are:

$$\dot{A}_3 = C_3^{-1}(f_1 - f_5 + f_{10} - f_{17} - f_{19}) \quad . . (82)$$

$$\dot{A}_6 = C_6^{-1} f_5 \quad . . . . . (83)$$

$$\dot{A}_{14} = C_{14}^{-1}(-f_{10} + f_{17}) \quad . . . . . (84)$$

$$\dot{A}_{25} = C_{25}^{-1}(-nf_{10} + f_{21} - f_{26}) \quad . . . . . (85)$$

$$f_5 = R_5^{-1}(A_3 - A_6) \quad . . . . . (86)$$

$$f_{10} = R_{10}^{-1}(-A_3 + A_{14} + nA_{25}) \quad . . . . . (87)$$

$$f_{17} = \alpha_{17} A_{25} \quad . . . . . (88)$$

$$f_{19} = \beta_{19} A_3 \quad . . . . . (89)$$

$$f_{21} = R_{21}^{-1}(A_{20} - A_{25}) \quad . . . . . (90)$$

$$f_{26} = R_{26}^{-1} A_{25} \quad . . . . . (91)$$

These component equations are presented in matrix form in Figure 11.

State Space Equations

The coefficient matrices in Figure 11 can be identified as the coefficient matrices (C_{ij}) in the general form of the matrix equations (Equation 17). The matrix equations in Figure 11 may be reduced to the state space form (Equation 16) by performing the operations indicated on page 22. The state equations which result from these operations are:

$$\dot{A}_3 = (-R_5^{-1}C_3^{-1} - R_{10}^{-1}C_3^{-1} - \beta_{19}C_3^{-1})A_3 + R_5^{-1}C_3^{-1}A_6 + R_{10}^{-1}C_3^{-1}A_{14} + (nR_{10}^{-1} - \alpha_{17})C_3^{-1}A_{25} \quad . . (92)$$

$$\dot{A}_6 = R_5^{-1}C_6^{-1}A_3 - R_5^{-1}C_6^{-1}A_6 \quad . . . . . (93)$$

$$\dot{A}_{14} = R_{10}^{-1}C_{14}^{-1}A_3 - R_{10}^{-1}C_{14}^{-1}A_{14} - (nR_{10}^{-1} - \alpha_{17})C_{14}^{-1}A_{25} \quad . . . . . (94)$$

$$\dot{A}_{25} = n^{-1}R_{10}^{-1}C_{25}^{-1} - n^{-1}R_{10}^{-1}C_{25}^{-1}A_{14} - (n^2R_{10}^{-1}C_{25}^{-1} + R_{21}^{-1}C_{25}^{-1} - R_{26}^{-1}C_{25}^{-1})A_{25} \quad . . . . . (95)$$

These equations are a mathematical description of the energy processes in the oxygen subsystem of the microcosm as they are represented in the bond graph (Figure 10).

$$\frac{d}{dt}\begin{bmatrix} A_3 \\ A_6 \\ A_{14} \\ A_{25} \end{bmatrix} = \begin{bmatrix} \searrow & & & \\ & \searrow & 0 & \\ & 0 & \searrow & \\ & & & \searrow \end{bmatrix} \begin{bmatrix} A_3 \\ A_6 \\ A_{14} \\ A_{25} \end{bmatrix} + \begin{bmatrix} -C_3^{-1} & C_3^{-1} & -C_3^{-1} & -C_3^{-1} & 0 & 0 \\ C_6^{-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & -C_{14}^{-1} & C_{14}^{-1} & 0 & 0 & 0 \\ 0 & -nC_{25}^{-1} & 0 & 0 & C_{25}^{-1} & -C_{25}^{-1} \end{bmatrix} \begin{bmatrix} f_5 \\ f_{10} \\ f_{17} \\ f_{19} \\ f_{21} \\ f_{26} \end{bmatrix} + \begin{bmatrix} C_3^{-1} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ A_{20} \end{bmatrix}$$

$$\begin{bmatrix} f_5 \\ f_{10} \\ f_{17} \\ f_{19} \\ f_{21} \\ f_{26} \end{bmatrix} = \begin{bmatrix} R_5^{-1} & -R_5^{-1} & 0 & 0 \\ -R_{10}^{-1} & 0 & R_{10}^{-1} & nR_{10}^{-1} \\ 0 & 0 & 0 & \alpha_{17} \\ \beta_{19} & 0 & 0 & 0 \\ 0 & 0 & 0 & -R_{21}^{-1} \\ 0 & 0 & 0 & R_{26}^{-1} \end{bmatrix} \begin{bmatrix} A_3 \\ A_6 \\ A_{14} \\ A_{25} \end{bmatrix} + \begin{bmatrix} \searrow & & & \\ & \searrow & 0 & \\ & 0 & \searrow & \\ & & & \searrow \end{bmatrix} \begin{bmatrix} f_5 \\ f_{10} \\ f_{17} \\ f_{19} \\ f_{21} \\ f_{26} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & R_{21}^{-1} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ A_{20} \end{bmatrix}$$

Figure 11. Matrix form of the component equations.

System Transfer Functions

The observable transfer function of the oxygen subsystem of the microcosm for each output may be obtained from the state equations of the system (Equations 92 through 95) and Equation 20. The transfer functions which result are:

$$H_3^*(s) = \frac{m}{s-a} + \frac{A_3(0)}{(s-a)\,U(s)} \quad \ldots\ldots\ldots (96)$$

$$H_6^*(s) = \frac{-bm}{(s-a)(s+b)} + \left(\frac{A_{14}(0)}{s+b} + \frac{A_3(0)C}{(s-a)(s+c)}\right) U(s)^{-1} \quad \ldots\ldots\ldots (97)$$

$$H_{14}^*(s) = \frac{P}{s+c} + \frac{mp}{(s-a)(s+c)} + \left(\frac{A_{14}(0)}{s+c} + \frac{A_3(0)C}{(s-a)(s+c)}\right) U(s)^{-1} \quad \ldots\ldots\ldots (98)$$

$$H_{25}^* = \frac{g}{s-e} + \frac{pd}{(s+c)(s-e)} + \frac{md}{(s-a)(s+c)} - \frac{mcd}{(s+a)(s+c)(s-b)} + \frac{dA_{14}(0)}{(s+c)(s-e)} - \frac{A_3(0)d}{(s-a)(s-e)} - \frac{A_3(0)\,dc}{(s-a)(s+c)(s-e)} U(s)^{-1} \quad \ldots\ldots\ldots (99)$$

in which $A_i(0)$ is the initial value of the state variable A_i and the following substitutions of component values should be observed.

$$a = -\beta_{19} C_3^{-1} \quad \ldots\ldots\ldots (100)$$

$$b = R_5^{-1} C_6^{-1} \quad \ldots\ldots\ldots (101)$$

$$c = R_{10}^{-1} C_{14}^{-1} (-n^2 R_{10}^{-1} - R_{21}^{-1} + R_{26}^{-1}) C_{25}^{-1} + nR_{10}^{-1} C_{25}^{-1} C_{14}^{-1} (nR_{10}^{-1} - \alpha_{17}) \quad \ldots\ldots\ldots (102)$$

$$d = n^{-1} R_{10}^{-1} C_{25}^{-1} \quad \ldots\ldots\ldots (103)$$

$$e = C_{25}^{-1} (-n^2 R_{10}^{-1} - R_{21}^{-1} + R_{26}^{-1}) \quad \ldots\ldots\ldots (104)$$

$$g = R_{21}^{-1} C_{25}^{-1} \quad \ldots\ldots\ldots\ldots \quad (105)$$

$$m = C_3^{-1} \quad \ldots\ldots\ldots\ldots \quad (106)$$

$$p = R_{21}^{-1} C_{25}^{-1} C_{14}^{-1} (nR_{10}^{-1} - \alpha_{17}) \quad \ldots \quad (107)$$

The observable transfer function for each output may also be obtained from the synthetic division of the output time series by the input time series (Figure 2) and Equation 21.

The time, mid-interval time, output, and the result of the synthetic division (h_a) for each output except water (A_{14}) which was assumed constant, are presented in Tables 7 through 9. Using the values of h_a and t from these tables in Equation 21 results in the following representations of the observable transfer functions.

$$H_3^*(s) = 2.17(10^{-5}) - 2.53(10^{-4})s \quad \ldots \quad (108)$$

$$H_6^*(s) = 3.39(10^{-5}) - 7.95(10^{-4})s + 6.82\,s^2 \quad \ldots\ldots\ldots \quad (109)$$

Table 7. Output data for dissolved oxygen (A_3) for the oxygen subsystem of the microcosm.

Time (Days)	Mid-Interval Time (Days)	Dissolved Oxygen Output A_3 (mg/l)	Synthetic Division Quotient h_a (mg/l)
28	14.0	12.8	12.8
36	32.0	14.7	1.9
43	39.5	15.0	0.3
50	46.5	14.6	-0.4
57	53.5	12.4	-2.2
64	60.5	16.2	3.7
71	67.5	13.6	-2.5
78	74.5	14.1	0.5
85	81.5	13.3	-0.8
92	88.5	14.5	1.2
99	95.5	13.5	-1.0
107	103.0	12.7	-0.8
113	109.0	13.9	1.2
120	116.5	11.9	-2.0
127	123.5	12.0	0.1
134	130.5	12.9	0.9
141	137.5	14.0	1.1
148	144.5	15.3	1.3
155	151.5	13.5	-1.8
162	158.5	12.8	-0.7

$$H_{14}^*(s) = 3.02(10^{-3}) - 2.11(10^{-2})s + 7.40(10^{-2})s^2 \quad \ldots\ldots\ldots \quad (110)$$

$$H_{25}^*(s) = 5.32(10^{-3}) + 1.32s \quad \ldots\ldots \quad (111)$$

Table 8. Output data for oxygen gas (A_6) for the oxygen subsystem of the microcosm.

Time (Days)	Mid-Interval Time (Days)	Oxygen Gas Output ($\%O_2$)	Synthetic Division Quotient h_a (mg/l)
7	3.5	19.8	19.8
14	10.5	25.5	5.7
28	21.0	45.1	19.6
43	35.5	39.2	-5.9
56	49.0	41.0	1.8
70	63.0	36.4	-4.6
84	77.0	36.4	0.0
98	91.0	42.2	5.8
111	104.5	41.4	-0.8
126	119.5	31.7	-9.7
140	133.0	40.3	8.6
154	147.0	43.0	2.7
168	161.0	43.0	0.0
182	175.0	43.0	0.0

Table 9. Output data for total organic carbon (A_{25}) for the oxygen subsystem of the microcosm.

Time (Days)	Mid-Interval Time (Days)	Organic Carbon (mg/l)	Synthetic Division Quotient h_a (mg/l)
14	7.0	4.0	4.0
28	21.0	6.5	2.5
42	36.0	16.0	9.5
56	49.0	13.0	-3.0
70	63.0	12.0	-1.0
84	77.0	7.5	-4.5
98	91.0	15.0	7.5
111	104.5	15.5	0.5
126	119.5	10.0	-5.5
140	133.0	3.0	-7.0
154	147.0	10.0	7.0
168	161.0	3.5	-6.5
182	175.0	3.5	0.0

Component Analysis

Some of the component values may be obtained mathematically by equating the two expressions for each transfer function (Equations 96 through 99 and 108 through 111). The other component values must be obtained either from measurement on the system or from the literature.

Equating the expression for $H_3^*(s)$ from Equation 96 with the expression for $H_3^*(s)$ from Equation 108 results in an equation with β_{19} and C_3 as the unknowns. The coefficients of like powers of s on each side of the equation must be equal so the following equations result:

$$C_3^{-1} = -2.17(10^{-5})\beta_{19}C_3^{-1} \quad \ldots\ldots (112)$$

$$\frac{(-3.02)(10^{-5})}{7.56} = (2.17)(10^{-5}) - (2.53)(10^{-4})\beta_{19}C_3^{-1} \quad \ldots\ldots\ldots (113)$$

These equations may be solved for β_{19} and C_3; the results are in Table 11.

Performing the same operations with the expressions for $H_6^*(s)$ gives:

$$\beta_{19} = -4.94(10^4) \quad \ldots\ldots\ldots (114)$$

$$R_5^{-1}C_6^{-1} = 7.46(10^{-2}) \quad \ldots\ldots (115)$$

Equation 115 can be used to determine either R_5 or C_6 once the other is known.

Equating the expressions for $H_{14}^*(s)$ and separating the equations for like coefficients results in two equations with n, R_{10}, C_{14}, α_{17}, R_{21}, C_{25}, and R_{26} as unknowns. Any two of the unknowns may be determined when the rest are known.

Finally, performing the same operations for $H_{25}^*(s)$ results with two equations with R_5, C_6, n, R_{10}, C_{14}, α_{17}, R_{21}, C_{25}, and R_{26} as unknowns. These two equations may be solved for two unknowns if the rest have been evaluated by other means.

The Capacitance Components

The capacitance values (C_3, C_6, C_{14}, and C_{25}) may be determined by analysis of the physical and chemical aspects of the processes of interest in the microcosms. The capacitance is related to the potential and the flux by the basic linear component equation,

$$I = C\frac{dE}{dt} \quad \ldots\ldots\ldots\ldots (3)$$

or

$$f = C\frac{dA}{dt} \quad \ldots\ldots\ldots\ldots (116)$$

Equation 116 indicates that the capacitance is equal to the reciprocal of the rate of change of potential per unit flux. The chemical potential (A) is related to the concentration of the chemical species ([Z]) by

$$A = A_o + RT \ln [Z] \quad \ldots\ldots\ldots (117)$$

in which A_o is the potential in a defined reference state, R is the universal gas constant, and T is the absolute temperature. The change in concentration is related to the flux and the volume over which the flux is distributed. Thus the rate of change of chemical potential is a logrithmic function of the flux and C must be based upon a linear approximation.

If the rate of change of the potential is evaluated using Equation 117 for a flux of 1 mg/day with an initial concentration midway between the extremes measured on the system then an approximate linear capacitance value may be determined. The approximate values are presented in Table 10.

The value in the table for biomass storage (C_{25}) is based upon measurements of organic carbon and there are some additional assumptions involved. It is assumed that organic carbon equals 50 percent of the dry weight (DiToro et al., 1971). It is also assumed that the dry weight equals 10 percent of the biomass (Morowitz, 1968).

One more component value is necessary in order to solve the equations resulting from $H_{14}^*(s)$ and $H_{25}^*(s)$ for the rest of the component values. α_{17} is the ratio of the flux of oxygen from dissolved oxygen into oxygen of water to the biomass potential. It is then the oxygen respiration rate. An average value of 1.13 (10^4) mg^2/Kcal-day at 25°C is assumed (DiToro et al., 1971).

Table 10. Reference potentials and capacitance values for the oxygen subsystem of the microcosm.

Storage of	Component	A_o (Kcal/mole)	Capacitance (mg^2/Kcal)
Dissolved O_2	C_3	3.9[a]	5.60×10^6
Gaseous O_2	C_6	0.0[b]	2.23×10^6
Water	C_{14}	-56.7[b]	2.98×10^9
Biomass	C_{25}	599.4[c]	5.95×10^3

The measured and derived component values are presented in Table 11.

System Analysis

The set of state space system equations (Equations 92 through 95) along with the component values constitutes a complete dynamic description of the system. These equations may be solved for the outputs as a function of time by analytical, analog computer, or digital computer techniques.

A digital computer program for solution of the system equations for the oxygen subsystem using the mimic system simulation language (see Stephenson, 1971) is presented in Appendix III.

Table 11. Measured and derived component and parameter values for the oxygen subsystem of the microcosm.

Component or Parameter	Measured Value	Derived Value
C_3	5.60 (10^6) mg^2/Kcal	4.52 (10^5) mg^2/Kcal
C_6	3.23 (10^6) mg^2/Kcal	-
C_{14}	2.98 (10^9) mg^2/Kcal	-
C_{25}	5.95 (10^3) mg^2/Kcal	-
R_5	-	4.15 (10^{-6}) Kcal-day/mg^2
R_{10}	-	2.35 (10^{-6}) Kcal-day/mg^2
R_{21}	-	2.37 (10^{-1}) Kcal-day/mg^2
R_{26}	-	2.41 (10^{-3}) Kcal-day/mg^2
α_{17}	1.13 (10^4) mg^2/Kcal/day	-
β_{19}	-	4.60 (10^4) mg^2/Kcal-day
$A_3(0)$	-3.02 (10^{-5}) Kcal/mg	-
$A_6(0)$	-2.98 (10^{-5}) Kcal/mg	-
$A_{14}(0)$	-3.02 (10^{-3}) Kcal/mg	-
$A_{25}(0)$	0.0 Kcal/mg	-
f_1	7.56 mg/day	-
n	5.80 (10^{-2})	-

The measured outputs and the result of the computer solution of the system equations are presented in Tables 12 through 14 and Figures 12 through 14. The poor replication of the carbon system is a direct result of the oversimplification of carbon dynamics in the microcosms (Figure 14).

Table 12. Observed and predicted values of dissolved oxygen concentration.

Observed Data		Predicted Data	
Time (Days)	D.O. (mg/l)	Time (Days)	D.O. (mg/l)
0	8.4	1	8.40
28	12.8	2	6.77
36	14.7	3	7.18
43	15.0	4	6.63
50	14.6	5	5.99
57	12.4	6	5.38
64	16.2	7	4.83
71	13.6	8	4.33
78	14.1	9	4.22
85	13.3	10	4.53
92	14.5	20	5.18
99	13.5	30	6.94
107	12.7	40	8.91
113	13.9	50	11.12
120	11.9	60	12.91
127	12.0	70	13.43
134	12.9	80	13.61
141	14.0	90	13.63
148	15.3	100	13.64
155	13.5	150	13.64
162	14.2	200	13.64
169	16.0		
176	14.2		

Table 13. Observed and predicted values of oxygen gas concentration.

Observed Data		Predicted Data	
Time (Days)	O_2 Percent	Time (Days)	O_2 Percent
7	19.8	0	20.0
14	25.5	5	25.2
28	45.1	10	26.0
43	39.2	20	28.2
56	41.0	30	32.6
70	36.4	40	37.1
84	36.4	50	39.0
98	42.2	60	39.6
111	41.4	70	39.8
126	31.7	80	39.9
140	40.3	90	39.9
154	43.0	100	39.9
168	43.0	150	39.9

Table 14. Observed and predicted values of organic carbon.

Observed Data		Predicted Data	
Time (Days)	Org C (mg/l)	Time (Days)	Org C (mg/l)
14	4.0	0	0.0
28	6.5	1	0.71
42	16.0	2	1.23
56	13.0	3	1.57
70	12.0	4	1.87
84	7.5	5	2.09
98	15.0	6	2.27
111	15.5	7	2.43
126	10.0	8	2.53
140	3.0	9	2.62
154	10.0	10	2.71
168	3.5	15	3.00
		20	3.14
		25	3.23
		30	3.30
		40	3.46
		50	3.49
		100	3.50
		150	3.50
		200	3.50

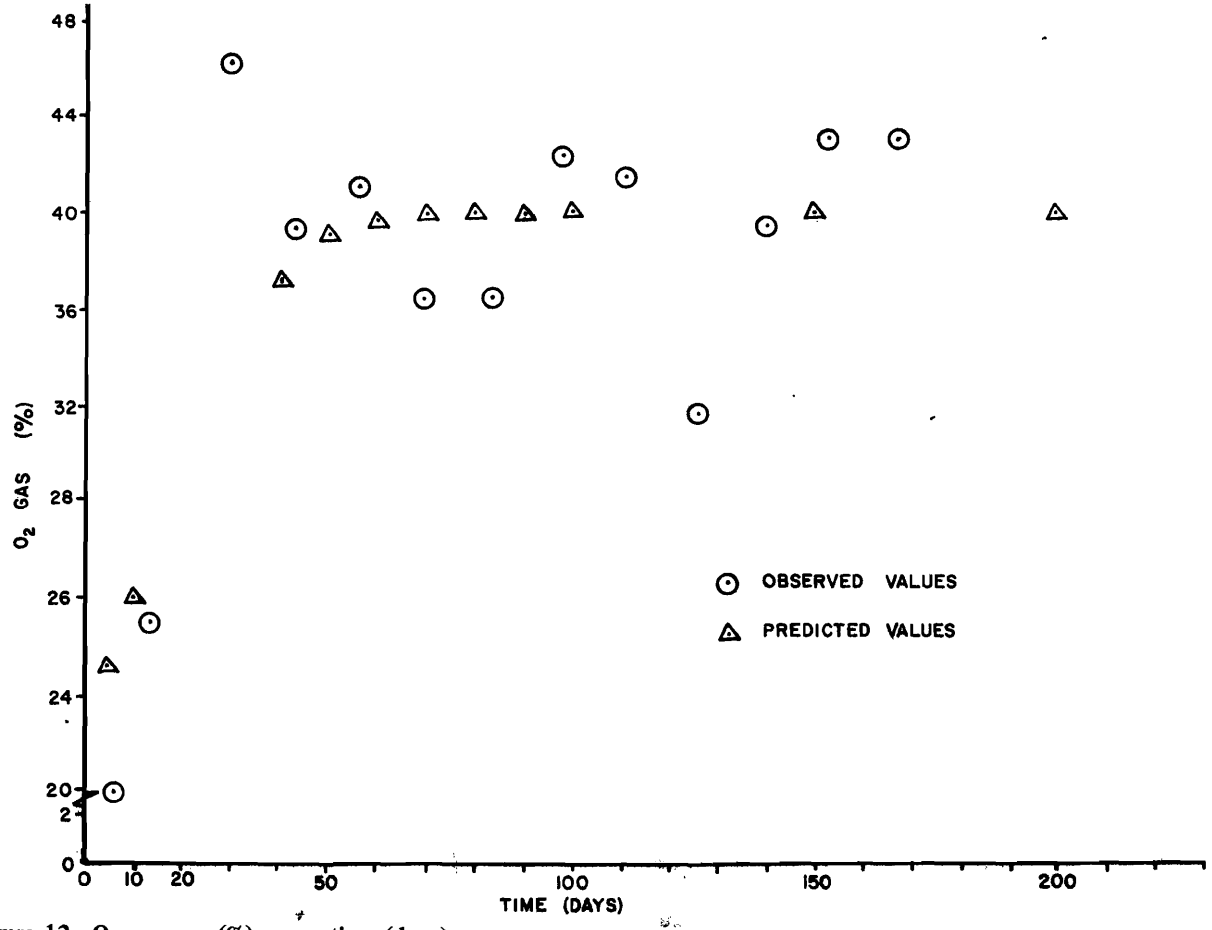


Figure 12. Oxygen gas (%) versus time (days).

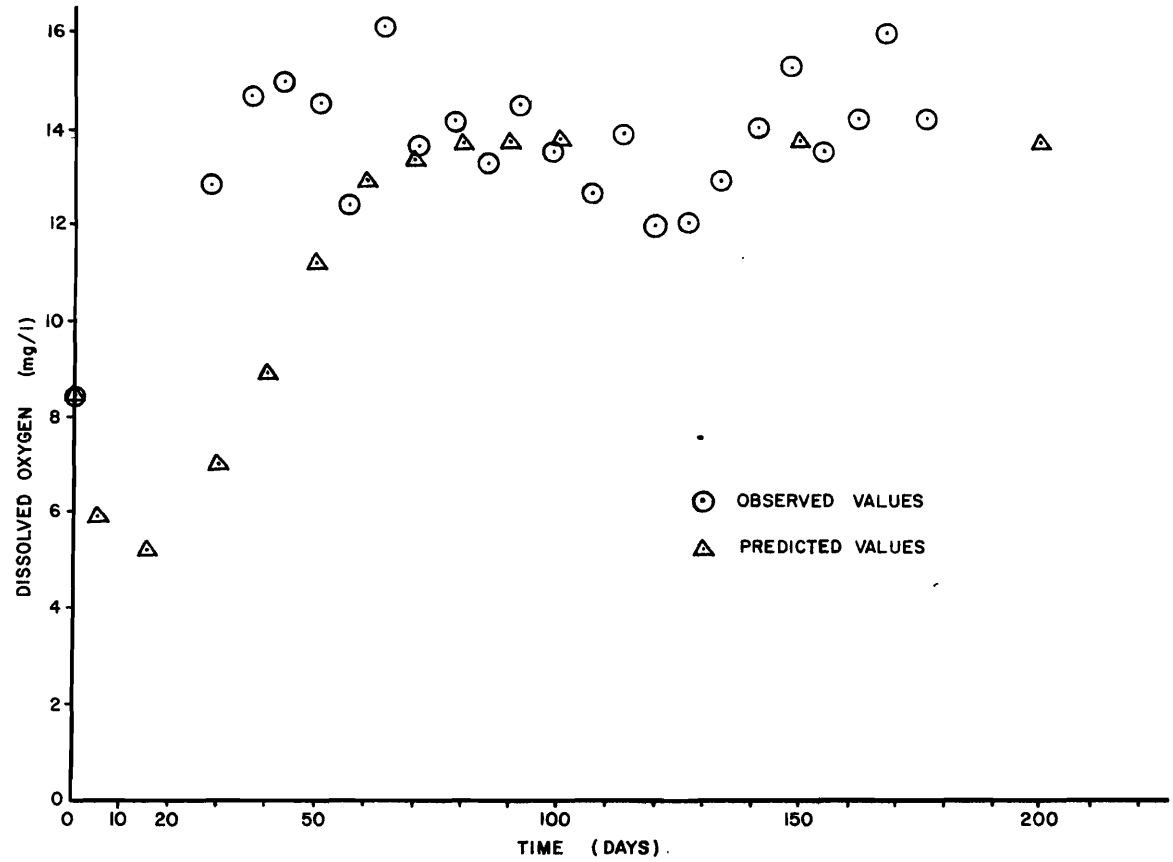


Figure 13. Dissolved oxygen (mg/l) versus time (days).

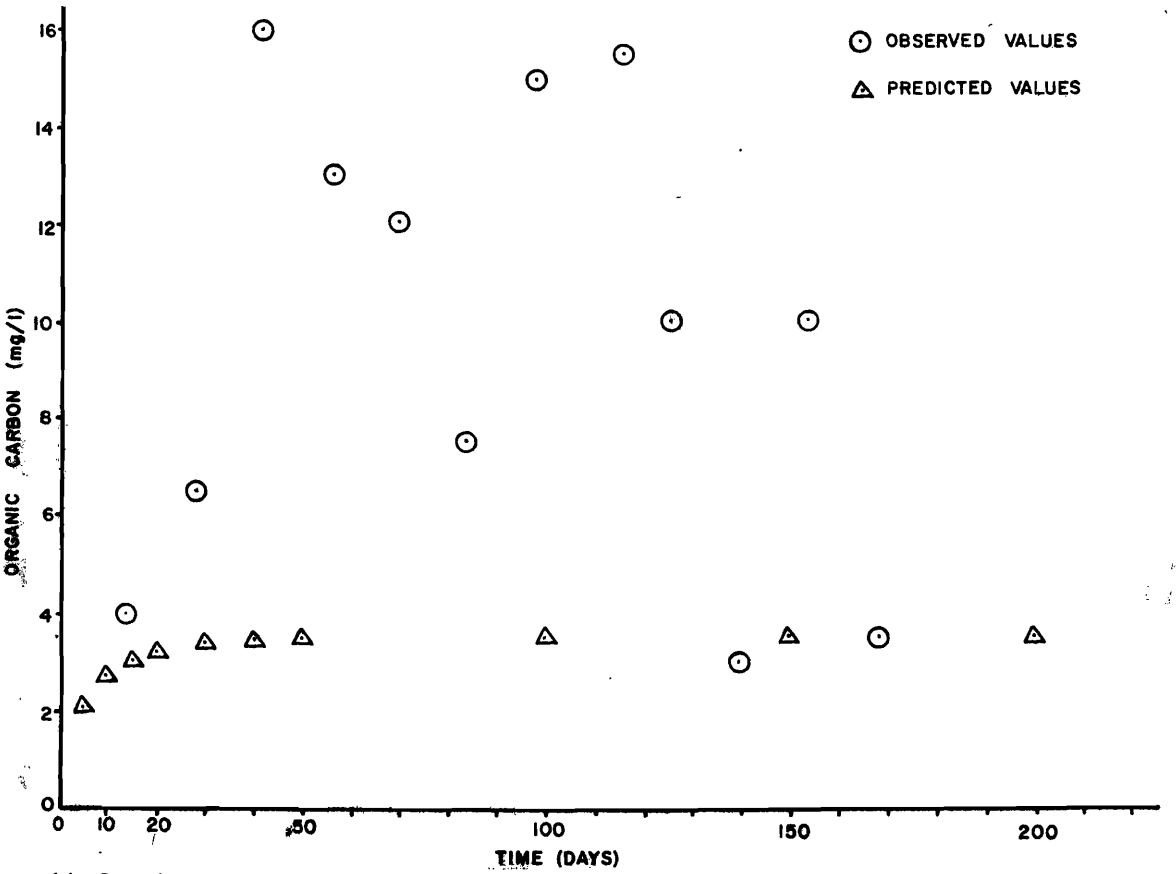


Figure 14. Organic carbon (mg/l) versus time (days).

DISCUSSION AND CONCLUSIONS

The analysis of the hydraulic system shows how well component analysis can be used to model physical processes when the energy processes are easily identified. The application of component analysis to the oxygen subsystem gives an indication of the difficulties encountered when many energy processes are involved in the physical process.

The accuracy of the model of the oxygen subsystem could be improved in many ways. One way would be to include some of the observed behavior of the system as inputs to the model. For example, the organic carbon concentration might be used to generate values for a time varying resistance to control the flux of oxygen due to photosynthesis and respiration.

A further extension of the preceding improvement might be to use the observed values of organic carbon as a time varying coefficient of a component to control oxygen flux due to respiration. In the same model, the observed values of relative fluorescence could be used as an input to a controlled oxygen flux source representing oxygen flux due to photosynthesis.

Each of the above improvements would probably increase the value of the model as a tool for prediction of system behavior. However, neither of the proposed improvements would increase the accuracy of the component values or the level of physical reality in the model. More complete analysis of the photosynthetic and respiratory oxygen components would be necessary to increase the accuracy of the model.

Enlarging Component Models

Including one of the energy processes which occur in the physical system in the model would involve redrawing the system bond graph and starting again from the component equations. The first model is an approximation and serves the purpose of showing that the technique is feasible. Also several of the component values will not change in a more complete representation of the oxygen subsystem. An example of a bond graph which includes light input (p_{30}) and separates autotrophs and heterotrophs is presented in Figure 15. The death rate, birth rate, respiration rate, and rate of photosynthesis of autotrophs and heterotrophs are isolated and represented by separate components in this model. A description of the components is presented in Table 15 and the component equations are listed in Table 16.

Continuation of these improvements to include components which represent individual species and coupling of the oxygen subsystem to the carbon dioxide or nitrogen subsystems is limited only by the time and effort necessary to complete the analysis and make the necessary measurements.

A major advantage of model improvement by addition of components or decomposition of previous components is that when a component value is determined for an isolated process then that component value is applicable to the same component in other models. Conversely, a major disadvantage of enlarged component models is the complexity of the mathematics involved in the component analysis.

Experimental Design

Component modeling and analysis has a big advantage when performed before the final design of an experiment. Prior to beginning a series of measurements and experiments on a biological or environmental system, an investigator can determine which measurements are important or necessary to complete the objectives of the study.

A cursory component analysis with a simple hypothesized graph structure can help to determine the minimum data necessary to characterize the system. If order of magnitude estimates are made for component values, then a simple sensitivity analysis will indicate which measurements are most critical in characterizing the system. Finally, time constants may be approximated from the estimated component values and structure and the frequency of measurements may be estimated.

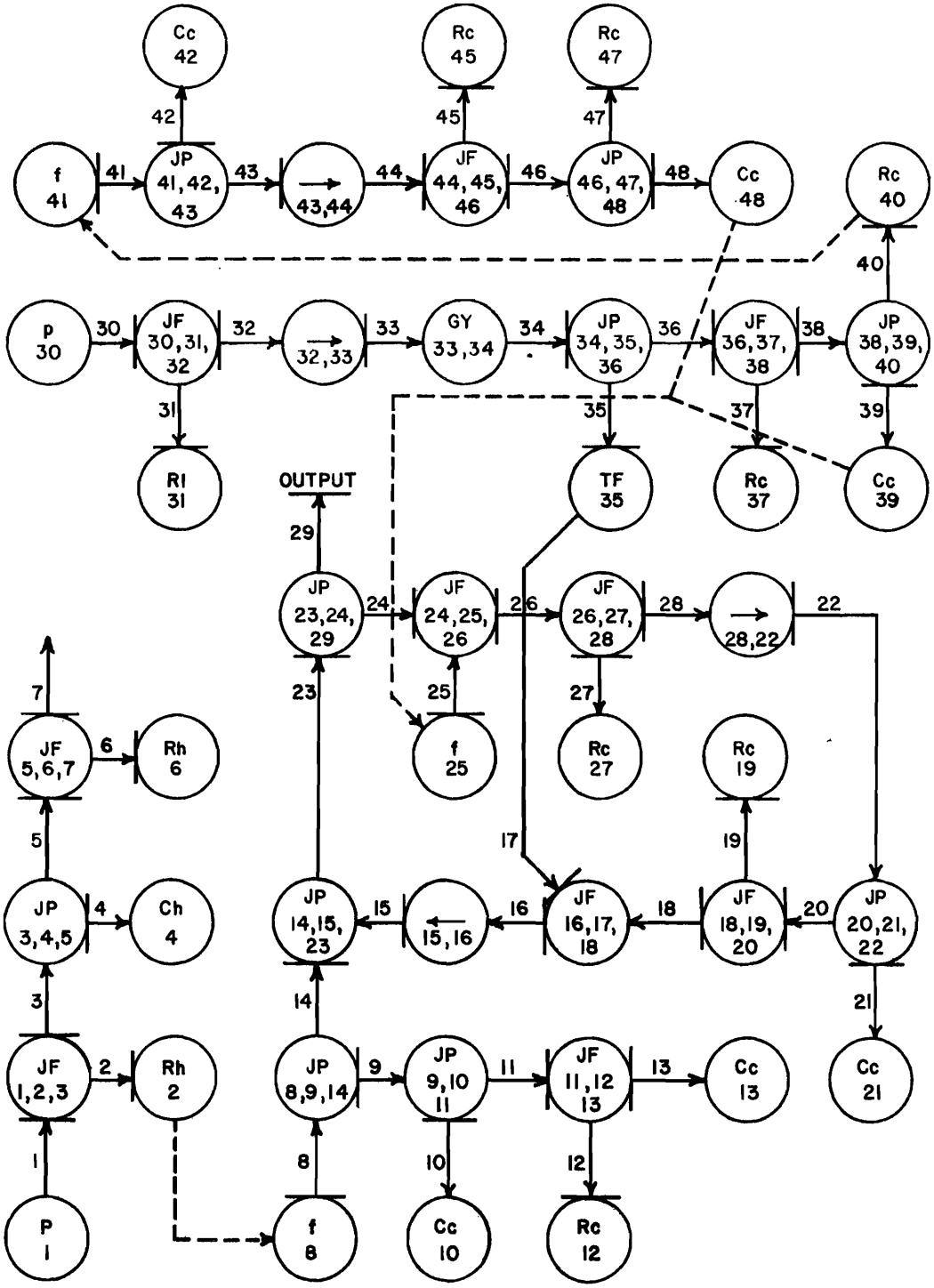


Figure 15. Bond graph of the oxygen subsystem with light input and separation of heterotrophs and autotrophs.

Table 15. Description of the components in Figure 15.

P_1	Hydraulic pressure source
Rh_2	Hydraulic resistance at input orifice
Ch_4	Hydraulic capacitance
Rh_6	Hydraulic resistance at output orifice
f_8	Oxygen flux source
Cc_{10}	Chemical capacitance for dissolved oxygen
Rc_{12}	Chemical resistance between liquid and gas
Cc_{13}	Chemical capacitance for oxygen gas
$R_{c\ 19}$	Chemical resistance to flow from water to dissolved oxygen
Cc_{21}	Chemical capacitance for water
f_{25}	Controlled flux source (respiration)
Rc_{27}	Chemical resistance to respiration
p_{30}	Light potential source
Rl_{31}	Light resistance of air and plastic
GY	Gyrator converting from light flux to chemical potential
TF	Transformer converting from autotroph production to oxygen release from water
Rc_{37}	Growth resistance of autotrophs
Cc_{39}	Chemical capacitance for storage of autotroph biomass
Rc_{40}	Decay resistance of autotrophs
f_{41}	Controlled chemical flux source from autotrophs to heterotrophs
Cc_{42}	Storage of dead autotrophs in water
Rc_{45}	Growth resistance of heterotrophs
Rc_{47}	Decay resistance of heterotrophs
Cc_{48}	Storage of chemical potential in heterotroph biomass.

Table 16. Component equations for bond graph of Figure 15.

$$\dot{P}_4 = Ch_4^{-1}(Q_2 - Q_6)$$

$$\dot{A}_{10} = Cc_{10}^{-1}(f_8 - f_{12} + f_{19} - f_{25} - f_{29})$$

$$\dot{A}_{13} = Cc_{13}^{-1}(f_{12})$$

$$\dot{A}_{21} = Cc_{21}^{-1}(-f_{19} + f_{25})$$

$$\dot{A}_{39} = Cc_{39}^{-1}(f_{37} - f_{40})$$

$$\dot{A}_{42} = Cc_{42}^{-1}(f_{41} - f_{45})$$

$$\dot{A}_{48} = Cc_{48}^{-1}(f_{45} - f_{47})$$

$$Q_2 = Rh_2^{-1}(P_1 - P_4)$$

$$Q_6 = Rh_6^{-1}(P_4)$$

$$f(8) = C_{28}^{1}(Q_2)$$

$$f_{12} = Rc_{12}^{-1}(A_{10} - A_{13})$$

$$f_{19} = Rc_{19}^{-1}(-A_{10} + A_{17} + A_{21})$$

$$f_{25} = C_{25,39}^{1}(A_{39}) + C_{25,48}(A_{48})$$

$$A_{27} = Rc_{27}(f_{25})$$

$$f_{29} = C_{29,6}^{1}(Q_6)$$

$$W_{31} = Rl_{31}^{-1}(P_{30} - P_{33})$$

$$f_{37} = Rc_{37}^{-1}(A_{34} - A_{39})$$

$$f_{40} = Rc_{40}^{-1}(A_{39})$$

$$f_{41} = C_{41,40}^{1}(f_{40})$$

$$f_{45} = Rc_{45}^{-1}(A_{42} - A_{48})$$

$$f_{47} = Rc_{47}^{-1}(A_{48})$$

$$P_{33} = M(f_{35} + f_{37})$$

$$A_{17} = n^{-1}(A_{34})$$

$$A_{34} = m(W_{31})$$

$$f_{35} = n^{-1}(f_{19})$$

GENERAL CONCLUSIONS

Component description of environmental systems is a detailed method of arriving at a system model which includes information concerning processes of energy transfer and transformation. The component analysis which is necessary if component values are not available or accessible for measurement, is tedious and expensive. The component values resulting from a component analysis are applicable to the same component in a similiar system therefore some component analyses need only be done once.

Component analysis can be applied to environmental systems. The stepwise sophistication of the conceptual model of the system and resultant component analysis will improve the generality of the output information. One major advantage of the modeling technique is the simultaneous modeling of energy and mass flow for the environmental system in question which is realistic in real systems. The approach was successfully applied to sediment-water microcosm experiments involving hydraulic flow and oxygen.

CITED LITERATURE

Astor, P. H., B. C. Patten, and J. Estberg. 1972. On sensitivity of ecosystem models. In: Project Reports: 1972 Summer Institute on the Systems Approach to the Life Sciences, Utah State University, Logan, Utah.

Ba Hli, F. 1971. A time domain approach. In: Aspects of Network and System Theory. Kalman, R.E., and N. DeClaris, ed. Holt, Rinehart, and Winston, New York, pp. 313-325.

Bertalanffy, L. von. 1968. General systems theory. George Braziller, Inc., New York, 289 p.

Boudart, M. 1968. Kinetics of chemical processes. Prentice-Hall, Inc., Englewood Cliffs, 246 p.

Callen, H. B. 1960. Thermodynamics. John Wiley and Sons, Inc., New York, p. 376.

Close, C. M. 1963. Notes on the analysis of linear circuits. Rensselaer Polytechnic Institute, Troy, 123 p.

Commoner, B. 1971. The closing circle. Alfred A. Knopf, Inc., New York, 326 p.

Daugherty, R. L., and J. B. Franzini. 1965 Fluid mechanics with engineering applications. McGraw-Hill, New York, 578 p.

DeGroot, S. R. 1963. Thermodynamics of irreversible processes. North-Holland Publishing Co., Amsterdam 242 p.

DeRusso, R. M., R. Roy, and C. Close. 1965. State variables for engineers. John Wiley and Sons, New York, p. 608.

Desoer, C. A. 1970. Notes for a second course on linear systems. Van Nostrand, Reinhold, New York, 199 p.

DiToro, D. M., D. J. O'Connor, and R. V. Thomann. 1971. A dynamic model of the phytoplankton in the Sacramento-San Joaquin Delta. In: Non-equilibrium systems in Natural Waters. ASC, Washington, D.C., pp. 131-180.

Fox, R. F. 1971. Entropy reduction in open systems. J. Theor. Biol., 31:43.

Karnopp, D., and R. C. Rosenberg. 1968. Analysis and simulation of multiport systems. M.I.T. Press, Cambridge, Mass., p. 221.

Katchalsky, A., and P. F. Curran. 1965. Non-equilibrium thermodynamics in biophysics. Harvard University Press, Cambridge, Mass., p. 248.

Kuo, B. C. 1962. Automatic control systems. Prentice-Hall, Englewood Cliffs, 504 p.

MacFarlane, A. G. J. 1964. Engineering systems analysis. Addison-Wesley, Reading, Mass., p. 272.

Martens, H. R., and O. R. Allen. 1969. Introduction to systems theory. C. E. Merrill Publishing Co., Columbus, 690 p.

Meadows, D. H., D. L. Meadows, J. Randers, W. H. Behrens III. 1972. The limits to growth. Universe Books, New York, 205 p.

Morowitz, H. J. 1968. Energy flow in biology. Academic Press, New York, 179 p.

Odum E. P. 1971. Fundamentals of ecology. Saunders, Philadelphia, 574 p.

Ogata, K. 1967. State space analysis of control systems. Prentice-Hall, Englewood Cliffs, 596 p.

Patten, B. C. 1972. Personal communication, N.S.F. Institute, Utah State University.

Porcella, D. B., K. L. Schmalz, and W. A. Luce. 1972. Sediment-water nutrient interchange in eutrophic lakes. Seminar on Eutrophication and Biostimulation, California Department of Water Resources, Sacramento, California. p. 83-109.

Porcella, D. B., V. D. Adams, P. A. Cowan, W. Holmes, S. Austrheim-Smith, J. Hill, IV, and E. J. Middlebrooks. 1973. Biological effects on interchange of metals and nutrients between sediments and water. OWRR Project Report, In Preparation, Utah Water Research Laboratory, Logan, Utah.

Prigogine, I. 1961. Introduction to thermodynamics of irreversible processes. Thomas, Springfield, Ill., p. 115.

Shearer, J. L., A. T. Murphy, and H. H. Richardson. 1967. Introduction to system dynamics. Addison-Wesley, Reading, 420 p.

Stephenson, R. E. 1971. Computer simulation for engineers. Harcourt Brace Jovanovich, Inc., New York, 504 p.

Taylor, S. A. 1963. Simultaneous flow in soils and plants. Utah State University, Logan, Utah. Var. p.

Tribus, M. 1961. Thermostatics and thermodynamics. Van Nostrand, New York, 500 p.

Wagman, D. D., et al. 1965. Selected values of chemical thermodynamic properties. Technical Note No. 270-1, N.B.S., U.S. Department of Commerce, Washington, D.C.

Walters, C. J. 1971. Systems ecology: The systems approach and mathematical models in ecology. In: Fundamentals of Ecology, by E. P. Odum, Saunders, Philadelphia, 574 p.

Weast, R. C. (ed.) 1970. Handbook of chemistry and physics. The Chemical Rubber Co., Cleveland.

SELECTED BIBLIOGRAPHY

Ashby, W. R. 1956. An introduction to cybernetics. Chapman and Hall, London, 295 p.

Caswell, H. 1972. An introduction to systems science for ecologists. To be published.

Conant, R. C. 1972. Detecting subsystems of a complex system. IEEE Transactions on Systems, Man, and Cybernetics, SMC2:551- 554.

DeGroot, S. R., and P. Mazur. 1962. Non-equilibrium thermodynamics. Interscience, New York, 510 p.

Forrester, J. W. 1971. World dynamics. Wright-Allen Press, Cambridge, Mass., p. 142.

Hall, D. J., et al. 1970. An experimental approach to the production dynamics and structure of fresh water animal communities. Limnol. Oceanog. 15:839.

Hatsopoulos, G. N., and J. H. Keenan. 1965. Principles of general thermodynamics. John Wiley and Sons, New York, p. 788.

Koenig, H. E., and R. L. Tummala. 1972. Principles of ecosystem design and management. IEEE Transactions on Systems, Man, and Cybernetics. SMC2:449.

Lehninger, A. L. 1965. Bioenergetics. W. A. Benjamin, Inc., New York, p. 258.

Linford, J. H. 1966. An introduction to energetics. Butterworths, London, p. 223.

Margalef, R. 1968. Perspectives in ecological theory. University of Chicago Press, Chicago, Illinois, 111 p.

Martinez, H. M. 1971. Morphogenesis and chemical dissipative structures. J. Theor. Biol. 36:139.

Mesarovic, M. D. 1968. Systems theory and biology. Springer-Verlag, New York, p. 403.

Milsum, J. H. 1966. Biological control systems. McGraw-Hill, New York, p. 566.

Odum, H. T. 1971. Environment, power, and society. John Wiley and Sons, New York, p. 331.

Patten, B. C. (ed.) 1971. Systems analysis and simulation in ecology. Academic Press, New York, 1:584.

Porcella, D. B., et al. 1970. Biological effects on sediment-water nutrient interchange. Journal of the Sanitary Engineering Division, Proceedings of A.S.C.E., 96:911.

Ryan, P. F. J. 1972. Information, entropy, and various systems. J. Theor. Biol. 36:139.

Schrödinger, E. 1956. What is life? Doubleday, New York, p. 263.

Sonntag, R. E., and G. J. Van Wylen. 1966. Fundamentals of statistical thermodynamics. John Wiley and Sons, New York, p. 370.

Szent-Györgyi, A. 1957. Bioenergetics. Academic Press, New York, p. 143.

Tykodi, R. J. 1967. Thermodynamics of steady states. MacMillan Co., New York, p. 217.

Ulanowicz, R. E. 1972. Mass and energy flow in closed ecosystems. J. Theor. Biol. 34:239-253.

Watt, K. E. F. 1966. Systems analysis in ecology. Academic Press, New York, p. 276.

APPENDICES

Appendix I

Definition of Symbols

a→z	=	intermediate variables in some calculations, used for convenience	m	=	gyrator ratio and mass
A,B,C,	=	coefficients in matrix equations	N	=	number of moles
A	=	chemical potential	n	=	transformer ratio and summation index
A_r	=	area	P	=	pressure
B	=	coefficient of viscous friction	Q	=	volume flow rate
C	=	a capacitance	q	=	electrical charge and weight flow rate
C_e	=	electrical capacitance	R	=	a resistance and the universal gas constant
d	=	diameter	r	=	the exchange rate of a chemical reaction at equilibrium
E	=	generalized potential	R_e	=	electrical resistance
e	=	electrical potential and the base of natural logrithms	R_p	=	pneumatic resistance
F	=	mechanical force	S	=	entropy
f	=	rate of change of extent of reaction (chemical flux)	s	=	complex frequency or Laplace variable
f(t)	=	a function of t	T	=	temporary variables in matrix component equations and absolute temperature
G	=	Gibb's free energy	t	=	time
g	=	acceleration due to gravity	TF	=	transformer component
GY	=	gyrator component	U	=	input variables and internal energy
H	=	auxiliary variables in matrix component equations	V	=	volume
			v	=	velocity
			X	=	state variables
h	=	height	x	=	distance
h_a	=	area under the impulse response curve	Y	=	output variables
H(s)	=	system function or transfer function	α	=	control ratio in oxygen system
$H^*(s)$	=	observable transfer function	β	=	outflow ratio in oxygen system
I	=	generalized flux	Π	=	3.14159
Id	=	identity matrix	ρ	=	density
i	=	electrical current and subscript index	ρ_o	=	average density
j	=	number of state variables in the system		=	extent of reaction
JF	=	flux junction component	τ	=	dummy variable of integration
JP	=	potential junction component	μ	=	viscosity
k	=	mechanical spring constant	ν	=	stoichiometric coefficient
L	=	an inertance	[ ]	=	a matrix
l	=	length	{ }	=	a time series
L_c	=	chemical inertance	Σ	=	a summation
L_e	=	electrical inertance	$\int$	=	an integral

Appendix II

Definition of Terms

bond graph = a systematic method of graphical representation of energy processes (Karnopp and Rosenberg, 1968).

capacitance = a component which is used to represent the storage of potential energy; also a measure of the capability to store potential energy.

causality = the process used to determine the independent variables in a bond graphical representation of a system; also the result of the process of determining the independent variables.

compartment = a pool (reservoir) of energy or nutrients (Walters, 1971).

complementary variables = pairs of variables (a potential and flux) which may be related mathematically to describe the energy processing function of a component.

component = a mathematical model of a physical process involving energy flow or transformation; also the graphic symbol representing a physical process.

energy = the capacity for doing work.

equilibrium = the state of dynamic balance between opposing forces, the state of maximum stability (Stumm and Morgan, 1970).

flux = a complementary variable which is operationally defined by the method of measurement. A flux may be measured at one point in a system and it is dependent upon the amount of matter in the system.

gyrator = a transfer component which transforms a flux into a potential and a potential into a flux (Shearer et al., 1967).

inertance = a component which is used to represent the storage of kinetic energy; also a measure of the capability to store kinetic energy.

isotropic = exhibiting equal physical properties in all directions (an isotrophic = not isotrophic).

microcosm = a miniature world, especially a miniature complete ecosystem.

model = a mathematical, graphical, physical, or verbal simplification of some aspect of the universe which may be interpreted as an approximation of reality.

potential = a complementary variable which is operationally defined by the method of measurement. A potential must be measured at two points one of which is a reference and it is independent of the amount of matter in the system.

power = the time rate of change of energy.

resistance = a component used to represent the dissipation (usually the loss to heat) of power due to opposition to the transfer or transformation of energy.

state = the smallest collection of properties which must be specified at a time $t = 0$ in order to predict the behavior of a system for any time $t \geq 0$ when the inputs for $t \geq 0$ are known (Ogata, 1967).

state space = a mathematical abstraction of three-dimensional (Euclidean) space in which the coordinates are the state variables.

state variable = the collection of properties which must be specified to define the state.

source = a component used to represent the input of energy from outside the selected system boundaries.

system = a set of interacting components.

transfer function = the ratio of the Laplace transform of the output of a system to the Laplace transform of the input when there is no initial stored energy.

transformer = a transfer component which transforms a potential into another potential of possibly different value and transforms a flux into another flux of possibly different value.

Appendix III

Mimic Source-Language Program

```
          PAR(C3,C6,C14,C25,R5,R10)
          PAR(A20,D19,R21,R26,ALPHA)
          PAR(IA3,IA6,IA14,IA25,F1)
N         .058
F5        R5*(A3-A6)
F10       MAX(R10*(A14-A3+N*(A20-A25))/(1.-N*N*R10/R21),0.)
F17       MAX(ALPHA*A25,0J
F19       ABS(B19*A3)
F26       R26*A25
A3DOT     C3*(F1-F5+F10-F17-F19)
A6DOT     C6*F5
A14DOT    C14*(-F10+F17)
A25DOT    C25*(N*F10-F26)
A3        INT(A3DOT,IA3)
A6        INT(A6DOT,IA6)
A14       INT(A14DOT,IA14)
A25       INT(A25DOT,IA25)
DAYS      T
DT        1.0
          FIN(T,162.0
          HDR(DAYS,A3,A6,A14,A25,)
          OUT(DAYS,A3,A6,A14,A25,)
          END
```